



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:10 AM BST

PDB ID : 2O82  
Title : Duplex DNA containing an abasic site with an opposite dC (beta anomer) in 5'-G\_AC-3' (10 structure ensemble and averaged structure)  
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Deposited on : 2006-12-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

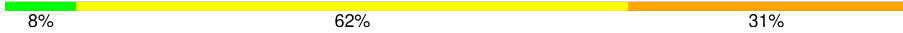

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric     | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|------------|-----------------------------|---------------------------|
| Clashscore | 114402                      | 11133                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain                                                                                                                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 13     | <br>8%                                              62%                                              31% |
| 2   | B     | 13     | <br>46%                                              54%                                                 |

## 2 Ensemble composition and analysis ⓘ

This entry contains 11 models. This entry does not contain protein, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 808 atoms, of which 291 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'.

| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
|     |       |          | Total | C   | H   | N  | O  | P  |       |
| 1   | A     | 13       | 399   | 121 | 142 | 52 | 72 | 12 | 0     |

- Molecule 2 is a DNA chain called 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'.


| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
|     |       |          | Total | C   | H   | N  | O  | P  |       |
| 2   | B     | 13       | 409   | 125 | 149 | 43 | 80 | 12 | 0     |

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A: 



- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

Chain B: 



### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A: 



- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

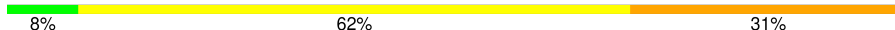
Chain B: 





#### 4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A:  8% 62% 31%




- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

Chain B:  38% 62%



#### 4.2.6 Score per residue for model 6

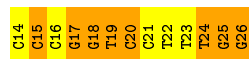
- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A:  8% 62% 31%



- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

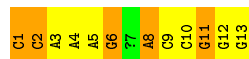
Chain B:  38% 62%



#### 4.2.7 Score per residue for model 7

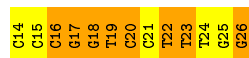
- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A:  8% 54% 38%



- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

Chain B:  38% 62%



### 4.2.8 Score per residue for model 8

- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A:  8% 38% 54%



- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

Chain B:  31% 69%



### 4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A:  8% 54% 38%



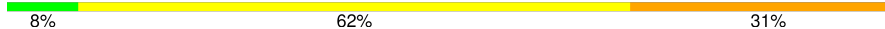
- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

Chain B:  62% 38%



### 4.2.10 Score per residue for model 10

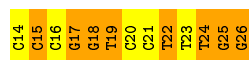
- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A:  8% 62% 31%



- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'


Chain B:  38% 62%






#### 4.2.11 Score per residue for model 11

- Molecule 1: 5'-D(\*CP\*CP\*AP\*AP\*AP\*GP\*(AAB)P\*AP\*CP\*CP\*GP\*GP\*G)-3'

Chain A:  23% 77%

|    |    |    |    |    |    |    |    |    |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|
| C1 | C2 | A3 | A4 | A5 | A6 | A7 | A8 | C9 | C10 | G11 | G12 | G13 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|

- Molecule 2: 5'-D(\*CP\*CP\*CP\*GP\*GP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*G)-3'

Chain B:  15% 85%

|     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C14 | C15 | C16 | G17 | G18 | T19 | C20 | C21 | T22 | T23 | T24 | G25 | G26 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing molecular dynamics matrix relaxation*.

Of the 30 calculated structures, 11 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|----------------|---------|
| Amber         | refinement     | 8.0     |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AAB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 3.22±0.51    | 34±11/275 (12.5±4.2%) | 4.11±0.54   | 80±20/420 (19.0±4.7%) |
| 2   | B     | 3.22±0.52    | 37±13/289 (12.9±4.3%) | 3.92±0.57   | 76±19/444 (17.1±4.3%) |
| All | All   | 3.26         | 790/6204 (12.7%)      | 4.05        | 1710/9504 (18.0%)     |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 4.8±2.2   |
| 2   | B     | 0.0±0.0   | 6.5±2.5   |
| All | All   | 0         | 124       |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|--------|-------------|----------|--------|-------|
|     |       |     |      |       |        |             |          | Worst  | Total |
| 2   | B     | 19  | DT   | C5-C7 | 16.41  | 1.59        | 1.50     | 5      | 5     |
| 1   | A     | 4   | DA   | N7-C5 | 14.54  | 1.48        | 1.39     | 2      | 2     |
| 1   | A     | 11  | DG   | N7-C5 | 14.41  | 1.47        | 1.39     | 2      | 6     |
| 2   | B     | 24  | DT   | C5-C7 | 14.38  | 1.58        | 1.50     | 10     | 8     |
| 1   | A     | 13  | DG   | N7-C5 | 13.53  | 1.47        | 1.39     | 6      | 3     |
| 2   | B     | 17  | DG   | N1-C2 | -13.23 | 1.27        | 1.37     | 6      | 3     |
| 2   | B     | 23  | DT   | C5-C7 | 13.00  | 1.57        | 1.50     | 8      | 7     |
| 1   | A     | 10  | DC   | N1-C6 | 12.96  | 1.45        | 1.37     | 4      | 5     |
| 1   | A     | 4   | DA   | N9-C4 | 12.66  | 1.45        | 1.37     | 8      | 1     |
| 2   | B     | 16  | DC   | N1-C6 | 12.59  | 1.44        | 1.37     | 3      | 2     |
| 1   | A     | 12  | DG   | N3-C4 | 12.51  | 1.44        | 1.35     | 8      | 4     |
| 1   | A     | 8   | DA   | N7-C5 | 11.99  | 1.46        | 1.39     | 8      | 4     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|--------|-------------|----------|--------|-------|
|     |       |     |      |         |        |             |          | Worst  | Total |
| 1   | A     | 10  | DC   | N3-C4   | -11.68 | 1.25        | 1.33     | 3      | 5     |
| 1   | A     | 13  | DG   | N3-C4   | 11.55  | 1.43        | 1.35     | 1      | 4     |
| 1   | A     | 2   | DC   | N1-C6   | 11.19  | 1.43        | 1.37     | 4      | 2     |
| 2   | B     | 15  | DC   | C4'-O4' | -11.16 | 1.33        | 1.45     | 3      | 2     |
| 2   | B     | 16  | DC   | N3-C4   | -11.04 | 1.26        | 1.33     | 6      | 3     |
| 2   | B     | 25  | DG   | P-O5'   | 10.93  | 1.70        | 1.59     | 2      | 3     |
| 2   | B     | 26  | DG   | N9-C4   | 10.86  | 1.46        | 1.38     | 9      | 3     |
| 2   | B     | 24  | DT   | N1-C2   | 10.83  | 1.46        | 1.38     | 6      | 5     |
| 2   | B     | 20  | DC   | N3-C4   | -10.47 | 1.26        | 1.33     | 9      | 1     |
| 2   | B     | 26  | DG   | P-O5'   | 10.46  | 1.70        | 1.59     | 2      | 4     |
| 1   | A     | 4   | DA   | P-O5'   | 10.38  | 1.70        | 1.59     | 3      | 5     |
| 2   | B     | 18  | DG   | C4'-O4' | -10.18 | 1.34        | 1.45     | 1      | 1     |
| 2   | B     | 24  | DT   | C4'-O4' | -10.10 | 1.34        | 1.45     | 2      | 4     |
| 2   | B     | 17  | DG   | C2-N2   | -10.03 | 1.24        | 1.34     | 8      | 3     |
| 1   | A     | 11  | DG   | C4'-C3' | 9.96   | 1.63        | 1.53     | 10     | 2     |
| 2   | B     | 25  | DG   | C2'-C1' | 9.96   | 1.62        | 1.52     | 4      | 3     |
| 2   | B     | 26  | DG   | N7-C5   | 9.89   | 1.45        | 1.39     | 10     | 4     |
| 2   | B     | 25  | DG   | C2-N2   | -9.88  | 1.24        | 1.34     | 10     | 2     |
| 1   | A     | 13  | DG   | C5'-C4' | 9.85   | 1.62        | 1.51     | 6      | 4     |
| 2   | B     | 15  | DC   | P-O5'   | 9.79   | 1.69        | 1.59     | 5      | 2     |
| 1   | A     | 6   | DG   | C4'-O4' | -9.79  | 1.35        | 1.45     | 2      | 4     |
| 2   | B     | 25  | DG   | N7-C5   | 9.78   | 1.45        | 1.39     | 3      | 5     |
| 1   | A     | 1   | DC   | O3'-P   | 9.74   | 1.72        | 1.61     | 1      | 1     |
| 2   | B     | 19  | DT   | C2-N3   | 9.74   | 1.45        | 1.37     | 6      | 2     |
| 2   | B     | 23  | DT   | O3'-P   | 9.73   | 1.72        | 1.61     | 6      | 4     |
| 2   | B     | 18  | DG   | C2-N2   | -9.70  | 1.24        | 1.34     | 1      | 4     |
| 1   | A     | 11  | DG   | C5-C4   | -9.67  | 1.31        | 1.38     | 10     | 2     |
| 2   | B     | 24  | DT   | C4-C5   | 9.65   | 1.53        | 1.45     | 8      | 2     |
| 2   | B     | 18  | DG   | P-O5'   | 9.64   | 1.69        | 1.59     | 3      | 2     |
| 2   | B     | 22  | DT   | C5-C6   | 9.64   | 1.41        | 1.34     | 5      | 5     |
| 2   | B     | 20  | DC   | C2-N3   | -9.62  | 1.28        | 1.35     | 6      | 1     |
| 2   | B     | 26  | DG   | N3-C4   | 9.57   | 1.42        | 1.35     | 3      | 5     |
| 1   | A     | 9   | DC   | C4'-O4' | -9.53  | 1.35        | 1.45     | 10     | 5     |
| 1   | A     | 12  | DG   | C6-N1   | -9.50  | 1.32        | 1.39     | 3      | 3     |
| 2   | B     | 22  | DT   | C5-C7   | 9.48   | 1.55        | 1.50     | 7      | 4     |
| 1   | A     | 3   | DA   | N7-C5   | 9.45   | 1.45        | 1.39     | 3      | 2     |
| 1   | A     | 12  | DG   | N9-C4   | 9.41   | 1.45        | 1.38     | 1      | 1     |
| 2   | B     | 19  | DT   | C5'-C4' | 9.40   | 1.61        | 1.51     | 1      | 3     |
| 1   | A     | 12  | DG   | O3'-P   | 9.39   | 1.72        | 1.61     | 4      | 3     |
| 2   | B     | 25  | DG   | N1-C2   | -9.32  | 1.30        | 1.37     | 7      | 4     |
| 1   | A     | 5   | DA   | N7-C5   | 9.32   | 1.44        | 1.39     | 10     | 6     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 2   | DC   | N3-C4   | -9.31 | 1.27        | 1.33     | 6      | 3     |
| 2   | B     | 14  | DC   | C2'-C1' | 9.31  | 1.61        | 1.52     | 4      | 2     |
| 1   | A     | 4   | DA   | N9-C8   | 9.31  | 1.45        | 1.37     | 1      | 1     |
| 2   | B     | 20  | DC   | P-O5'   | 9.07  | 1.68        | 1.59     | 5      | 2     |
| 1   | A     | 4   | DA   | N3-C4   | 9.05  | 1.40        | 1.34     | 6      | 8     |
| 1   | A     | 11  | DG   | N9-C4   | -9.02 | 1.30        | 1.38     | 1      | 3     |
| 1   | A     | 11  | DG   | N3-C4   | 8.95  | 1.41        | 1.35     | 6      | 7     |
| 2   | B     | 26  | DG   | N9-C8   | -8.79 | 1.31        | 1.37     | 5      | 2     |
| 1   | A     | 10  | DC   | C4-N4   | -8.78 | 1.26        | 1.33     | 10     | 4     |
| 1   | A     | 4   | DA   | C6-N1   | -8.78 | 1.29        | 1.35     | 3      | 4     |
| 1   | A     | 10  | DC   | C4'-C3' | 8.74  | 1.62        | 1.53     | 9      | 4     |
| 1   | A     | 5   | DA   | N3-C4   | 8.72  | 1.40        | 1.34     | 6      | 5     |
| 2   | B     | 17  | DG   | P-O5'   | 8.72  | 1.68        | 1.59     | 9      | 4     |
| 1   | A     | 12  | DG   | C8-N7   | 8.70  | 1.36        | 1.30     | 5      | 1     |
| 1   | A     | 11  | DG   | P-O5'   | 8.70  | 1.68        | 1.59     | 8      | 4     |
| 1   | A     | 9   | DC   | C4-N4   | -8.70 | 1.26        | 1.33     | 2      | 2     |
| 2   | B     | 24  | DT   | P-O5'   | 8.65  | 1.68        | 1.59     | 1      | 2     |
| 1   | A     | 6   | DG   | N3-C4   | 8.56  | 1.41        | 1.35     | 7      | 3     |
| 1   | A     | 13  | DG   | C6-N1   | 8.55  | 1.45        | 1.39     | 2      | 4     |
| 2   | B     | 17  | DG   | N7-C5   | 8.54  | 1.44        | 1.39     | 9      | 6     |
| 1   | A     | 3   | DA   | N3-C4   | 8.47  | 1.40        | 1.34     | 4      | 6     |
| 2   | B     | 22  | DT   | N1-C2   | 8.43  | 1.44        | 1.38     | 7      | 4     |
| 1   | A     | 4   | DA   | C5-C6   | 8.43  | 1.48        | 1.41     | 9      | 2     |
| 2   | B     | 23  | DT   | N3-C4   | -8.43 | 1.31        | 1.38     | 5      | 3     |
| 2   | B     | 14  | DC   | N1-C6   | 8.42  | 1.42        | 1.37     | 3      | 4     |
| 1   | A     | 13  | DG   | C4'-O4' | -8.38 | 1.36        | 1.45     | 6      | 3     |
| 1   | A     | 8   | DA   | N9-C4   | -8.37 | 1.32        | 1.37     | 1      | 2     |
| 2   | B     | 15  | DC   | C4-N4   | -8.35 | 1.26        | 1.33     | 10     | 6     |
| 1   | A     | 2   | DC   | C4'-C3' | 8.31  | 1.61        | 1.53     | 5      | 1     |
| 2   | B     | 16  | DC   | C2-N3   | 8.31  | 1.42        | 1.35     | 10     | 3     |
| 2   | B     | 15  | DC   | C5'-C4' | 8.29  | 1.60        | 1.51     | 8      | 2     |
| 1   | A     | 11  | DG   | C5'-C4' | 8.28  | 1.60        | 1.51     | 2      | 2     |
| 1   | A     | 12  | DG   | P-O5'   | 8.27  | 1.68        | 1.59     | 1      | 4     |
| 2   | B     | 16  | DC   | C4'-O4' | -8.25 | 1.36        | 1.45     | 8      | 1     |
| 2   | B     | 16  | DC   | C4-N4   | -8.16 | 1.26        | 1.33     | 4      | 2     |
| 2   | B     | 24  | DT   | C3'-C2' | 8.16  | 1.62        | 1.52     | 10     | 4     |
| 1   | A     | 1   | DC   | C4-N4   | -8.14 | 1.26        | 1.33     | 6      | 2     |
| 2   | B     | 16  | DC   | P-O5'   | 8.13  | 1.67        | 1.59     | 3      | 4     |
| 1   | A     | 4   | DA   | O3'-P   | 8.11  | 1.70        | 1.61     | 4      | 1     |
| 2   | B     | 26  | DG   | C4'-O4' | -8.10 | 1.36        | 1.45     | 5      | 2     |
| 1   | A     | 12  | DG   | N7-C5   | 8.07  | 1.44        | 1.39     | 7      | 3     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 2   | B     | 20  | DC   | N1-C6   | 8.05  | 1.42        | 1.37     | 10     | 3     |
| 2   | B     | 19  | DT   | C5-C6   | 8.02  | 1.40        | 1.34     | 5      | 5     |
| 1   | A     | 8   | DA   | C2'-C1' | 7.99  | 1.60        | 1.52     | 3      | 3     |
| 1   | A     | 12  | DG   | C4'-O4' | -7.98 | 1.37        | 1.45     | 5      | 6     |
| 1   | A     | 13  | DG   | C5-C6   | 7.92  | 1.50        | 1.42     | 8      | 1     |
| 1   | A     | 3   | DA   | C5-C4   | -7.92 | 1.33        | 1.38     | 1      | 2     |
| 2   | B     | 24  | DT   | N3-C4   | -7.92 | 1.32        | 1.38     | 8      | 4     |
| 1   | A     | 6   | DG   | C2-N2   | -7.91 | 1.26        | 1.34     | 8      | 6     |
| 2   | B     | 25  | DG   | C5'-C4' | 7.90  | 1.60        | 1.51     | 9      | 1     |
| 1   | A     | 3   | DA   | C6-N1   | -7.90 | 1.30        | 1.35     | 10     | 1     |
| 1   | A     | 2   | DC   | C2-N3   | -7.88 | 1.29        | 1.35     | 7      | 3     |
| 2   | B     | 26  | DG   | C2'-C1' | 7.87  | 1.60        | 1.52     | 6      | 3     |
| 2   | B     | 14  | DC   | C4'-C3' | 7.86  | 1.61        | 1.53     | 10     | 2     |
| 2   | B     | 14  | DC   | C2-O2   | -7.83 | 1.17        | 1.24     | 10     | 3     |
| 2   | B     | 21  | DC   | C4'-O4' | -7.81 | 1.37        | 1.45     | 5      | 2     |
| 2   | B     | 22  | DT   | C2-N3   | -7.80 | 1.31        | 1.37     | 10     | 2     |
| 2   | B     | 18  | DG   | C4'-C3' | 7.79  | 1.61        | 1.53     | 5      | 1     |
| 1   | A     | 11  | DG   | C8-N7   | 7.78  | 1.35        | 1.30     | 9      | 1     |
| 2   | B     | 19  | DT   | N1-C2   | 7.75  | 1.44        | 1.38     | 3      | 3     |
| 2   | B     | 15  | DC   | N1-C6   | 7.74  | 1.41        | 1.37     | 7      | 2     |
| 1   | A     | 9   | DC   | C1'-N1  | 7.74  | 1.59        | 1.49     | 2      | 1     |
| 1   | A     | 12  | DG   | C4'-C3' | 7.74  | 1.61        | 1.53     | 4      | 2     |
| 2   | B     | 15  | DC   | C4-C5   | -7.70 | 1.36        | 1.43     | 5      | 1     |
| 1   | A     | 10  | DC   | O4'-C1' | 7.69  | 1.51        | 1.42     | 9      | 3     |
| 2   | B     | 18  | DG   | C3'-O3' | 7.69  | 1.53        | 1.44     | 1      | 1     |
| 1   | A     | 6   | DG   | C5'-C4' | 7.67  | 1.59        | 1.51     | 9      | 2     |
| 1   | A     | 10  | DC   | C5'-C4' | 7.67  | 1.59        | 1.51     | 3      | 4     |
| 2   | B     | 14  | DC   | N1-C2   | 7.61  | 1.47        | 1.40     | 3      | 1     |
| 1   | A     | 2   | DC   | C4'-O4' | -7.58 | 1.37        | 1.45     | 9      | 2     |
| 2   | B     | 24  | DT   | C2-O2   | 7.56  | 1.28        | 1.22     | 9      | 3     |
| 2   | B     | 21  | DC   | N1-C6   | 7.53  | 1.41        | 1.37     | 4      | 2     |
| 1   | A     | 10  | DC   | N1-C2   | 7.53  | 1.47        | 1.40     | 10     | 3     |
| 1   | A     | 13  | DG   | P-O5'   | -7.51 | 1.52        | 1.59     | 8      | 3     |
| 1   | A     | 9   | DC   | N1-C6   | 7.48  | 1.41        | 1.37     | 6      | 1     |
| 1   | A     | 6   | DG   | C5-C6   | 7.48  | 1.49        | 1.42     | 4      | 2     |
| 1   | A     | 5   | DA   | C5-C4   | -7.47 | 1.33        | 1.38     | 8      | 3     |
| 2   | B     | 18  | DG   | N3-C4   | 7.46  | 1.40        | 1.35     | 6      | 2     |
| 2   | B     | 17  | DG   | N3-C4   | 7.45  | 1.40        | 1.35     | 2      | 4     |
| 2   | B     | 16  | DC   | O3'-P   | 7.44  | 1.70        | 1.61     | 1      | 3     |
| 2   | B     | 21  | DC   | O3'-P   | 7.44  | 1.70        | 1.61     | 9      | 3     |
| 2   | B     | 22  | DT   | O3'-P   | 7.44  | 1.70        | 1.61     | 10     | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 11  | DG   | C2-N2   | -7.44 | 1.27        | 1.34     | 4      | 5     |
| 1   | A     | 12  | DG   | C5-C4   | 7.39  | 1.43        | 1.38     | 1      | 3     |
| 2   | B     | 26  | DG   | C8-N7   | 7.39  | 1.35        | 1.30     | 9      | 2     |
| 2   | B     | 20  | DC   | C4'-O4' | -7.39 | 1.37        | 1.45     | 1      | 3     |
| 1   | A     | 6   | DG   | N7-C5   | 7.37  | 1.43        | 1.39     | 9      | 2     |
| 2   | B     | 20  | DC   | C5-C6   | 7.36  | 1.40        | 1.34     | 2      | 3     |
| 1   | A     | 4   | DA   | C8-N7   | -7.35 | 1.26        | 1.31     | 9      | 2     |
| 2   | B     | 24  | DT   | C5-C6   | 7.33  | 1.39        | 1.34     | 3      | 4     |
| 2   | B     | 16  | DC   | C4-C5   | 7.32  | 1.48        | 1.43     | 4      | 3     |
| 2   | B     | 14  | DC   | C4'-O4' | -7.29 | 1.37        | 1.45     | 4      | 2     |
| 1   | A     | 10  | DC   | C2-N3   | 7.27  | 1.41        | 1.35     | 1      | 3     |
| 2   | B     | 22  | DT   | C4'-O4' | -7.25 | 1.37        | 1.45     | 4      | 3     |
| 1   | A     | 13  | DG   | N9-C8   | 7.23  | 1.43        | 1.37     | 9      | 2     |
| 2   | B     | 23  | DT   | C2-O2   | 7.22  | 1.28        | 1.22     | 3      | 2     |
| 1   | A     | 3   | DA   | N9-C4   | -7.21 | 1.33        | 1.37     | 8      | 2     |
| 1   | A     | 1   | DC   | C2-O2   | -7.21 | 1.18        | 1.24     | 6      | 2     |
| 1   | A     | 4   | DA   | C5-C4   | -7.21 | 1.33        | 1.38     | 4      | 2     |
| 1   | A     | 5   | DA   | C6-N1   | -7.21 | 1.30        | 1.35     | 8      | 4     |
| 2   | B     | 26  | DG   | C6-N1   | -7.19 | 1.34        | 1.39     | 4      | 4     |
| 1   | A     | 2   | DC   | C4-N4   | -7.19 | 1.27        | 1.33     | 9      | 2     |
| 1   | A     | 6   | DG   | N9-C4   | 7.18  | 1.43        | 1.38     | 6      | 2     |
| 1   | A     | 8   | DA   | N3-C4   | 7.16  | 1.39        | 1.34     | 8      | 4     |
| 1   | A     | 9   | DC   | C5-C6   | 7.16  | 1.40        | 1.34     | 4      | 2     |
| 1   | A     | 8   | DA   | C6-N6   | -7.12 | 1.28        | 1.33     | 5      | 2     |
| 1   | A     | 12  | DG   | C5-C6   | 7.11  | 1.49        | 1.42     | 5      | 4     |
| 1   | A     | 3   | DA   | C8-N7   | 7.08  | 1.36        | 1.31     | 1      | 1     |
| 1   | A     | 5   | DA   | C6-N6   | -7.08 | 1.28        | 1.33     | 5      | 3     |
| 1   | A     | 1   | DC   | C4'-O4' | -7.08 | 1.38        | 1.45     | 5      | 2     |
| 1   | A     | 8   | DA   | C6-N1   | 7.02  | 1.40        | 1.35     | 4      | 1     |
| 2   | B     | 14  | DC   | O3'-P   | -7.01 | 1.52        | 1.61     | 4      | 3     |
| 1   | A     | 6   | DG   | P-O5'   | -7.01 | 1.52        | 1.59     | 6      | 3     |
| 1   | A     | 6   | DG   | C4'-C3' | 7.01  | 1.60        | 1.53     | 3      | 1     |
| 2   | B     | 23  | DT   | C3'-O3' | -7.01 | 1.34        | 1.44     | 9      | 1     |
| 1   | A     | 13  | DG   | N1-C2   | -6.99 | 1.32        | 1.37     | 2      | 4     |
| 2   | B     | 21  | DC   | C4-N4   | -6.99 | 1.27        | 1.33     | 9      | 3     |
| 1   | A     | 11  | DG   | C6-N1   | -6.98 | 1.34        | 1.39     | 1      | 2     |
| 2   | B     | 21  | DC   | C5'-C4' | 6.97  | 1.59        | 1.51     | 5      | 2     |
| 1   | A     | 3   | DA   | P-O5'   | 6.96  | 1.66        | 1.59     | 1      | 2     |
| 1   | A     | 11  | DG   | C5-C6   | 6.95  | 1.49        | 1.42     | 8      | 3     |
| 1   | A     | 12  | DG   | C5'-C4' | 6.94  | 1.58        | 1.51     | 1      | 3     |
| 2   | B     | 26  | DG   | C6-O6   | -6.93 | 1.18        | 1.24     | 3      | 4     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 8   | DA   | C5'-C4' | 6.93  | 1.58        | 1.51     | 7      | 2     |
| 2   | B     | 18  | DG   | C5'-C4' | 6.92  | 1.58        | 1.51     | 3      | 3     |
| 2   | B     | 21  | DC   | C2-O2   | -6.91 | 1.18        | 1.24     | 7      | 1     |
| 2   | B     | 20  | DC   | C4-N4   | -6.91 | 1.27        | 1.33     | 9      | 3     |
| 1   | A     | 13  | DG   | C2-N2   | -6.89 | 1.27        | 1.34     | 8      | 3     |
| 1   | A     | 2   | DC   | P-O5'   | 6.87  | 1.66        | 1.59     | 6      | 1     |
| 1   | A     | 2   | DC   | C4-C5   | -6.86 | 1.37        | 1.43     | 6      | 2     |
| 1   | A     | 9   | DC   | C2-N3   | -6.82 | 1.30        | 1.35     | 5      | 1     |
| 2   | B     | 25  | DG   | C4'-C3' | 6.81  | 1.60        | 1.53     | 4      | 3     |
| 2   | B     | 22  | DT   | P-O5'   | 6.80  | 1.66        | 1.59     | 7      | 2     |
| 1   | A     | 9   | DC   | P-O5'   | 6.80  | 1.66        | 1.59     | 2      | 5     |
| 1   | A     | 4   | DA   | C6-N6   | -6.78 | 1.28        | 1.33     | 8      | 3     |
| 2   | B     | 26  | DG   | C5-C4   | 6.76  | 1.43        | 1.38     | 7      | 4     |
| 2   | B     | 23  | DT   | C4'-O4' | -6.73 | 1.38        | 1.45     | 10     | 3     |
| 1   | A     | 1   | DC   | N1-C6   | 6.72  | 1.41        | 1.37     | 3      | 2     |
| 2   | B     | 23  | DT   | N1-C2   | 6.71  | 1.43        | 1.38     | 2      | 1     |
| 2   | B     | 14  | DC   | C5'-C4' | 6.70  | 1.58        | 1.51     | 1      | 1     |
| 1   | A     | 1   | DC   | N3-C4   | -6.69 | 1.29        | 1.33     | 8      | 4     |
| 2   | B     | 18  | DG   | O3'-P   | 6.68  | 1.69        | 1.61     | 2      | 2     |
| 2   | B     | 17  | DG   | N9-C8   | -6.68 | 1.33        | 1.37     | 10     | 3     |
| 1   | A     | 10  | DC   | O3'-P   | -6.67 | 1.53        | 1.61     | 7      | 1     |
| 2   | B     | 21  | DC   | O4'-C1' | 6.65  | 1.50        | 1.42     | 1      | 2     |
| 2   | B     | 22  | DT   | C2-O2   | 6.62  | 1.27        | 1.22     | 7      | 3     |
| 2   | B     | 18  | DG   | C6-N1   | -6.62 | 1.34        | 1.39     | 6      | 2     |
| 1   | A     | 13  | DG   | C2-N3   | 6.60  | 1.38        | 1.32     | 9      | 1     |
| 1   | A     | 13  | DG   | N9-C4   | -6.58 | 1.32        | 1.38     | 3      | 1     |
| 2   | B     | 26  | DG   | C5'-C4' | 6.56  | 1.58        | 1.51     | 9      | 3     |
| 2   | B     | 25  | DG   | N3-C4   | 6.55  | 1.40        | 1.35     | 5      | 3     |
| 2   | B     | 15  | DC   | C4'-C3' | -6.55 | 1.46        | 1.52     | 6      | 2     |
| 1   | A     | 4   | DA   | C2'-C1' | -6.55 | 1.45        | 1.52     | 8      | 1     |
| 2   | B     | 25  | DG   | C6-O6   | -6.53 | 1.18        | 1.24     | 9      | 2     |
| 1   | A     | 13  | DG   | C8-N7   | 6.52  | 1.34        | 1.30     | 6      | 2     |
| 2   | B     | 18  | DG   | N1-C2   | -6.49 | 1.32        | 1.37     | 7      | 1     |
| 1   | A     | 5   | DA   | C8-N7   | -6.49 | 1.27        | 1.31     | 7      | 1     |
| 2   | B     | 19  | DT   | N3-C4   | -6.44 | 1.33        | 1.38     | 5      | 2     |
| 1   | A     | 3   | DA   | C6-N6   | -6.42 | 1.28        | 1.33     | 6      | 5     |
| 1   | A     | 9   | DC   | C3'-C2' | 6.42  | 1.59        | 1.52     | 3      | 1     |
| 2   | B     | 26  | DG   | C2-N3   | 6.41  | 1.37        | 1.32     | 4      | 1     |
| 1   | A     | 10  | DC   | C4-C5   | -6.39 | 1.37        | 1.43     | 4      | 1     |
| 2   | B     | 25  | DG   | C8-N7   | 6.38  | 1.34        | 1.30     | 3      | 2     |
| 1   | A     | 4   | DA   | C5'-C4' | 6.37  | 1.58        | 1.51     | 4      | 3     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 2   | B     | 23  | DT   | C4-C5   | 6.36  | 1.50        | 1.45     | 4      | 2     |
| 1   | A     | 6   | DG   | C5-C4   | -6.35 | 1.33        | 1.38     | 1      | 2     |
| 1   | A     | 5   | DA   | C4'-O4' | -6.31 | 1.38        | 1.45     | 3      | 2     |
| 1   | A     | 1   | DC   | N1-C2   | 6.31  | 1.46        | 1.40     | 6      | 1     |
| 2   | B     | 23  | DT   | C5-C6   | 6.31  | 1.38        | 1.34     | 10     | 1     |
| 2   | B     | 17  | DG   | C4'-C3' | 6.28  | 1.59        | 1.53     | 3      | 1     |
| 2   | B     | 21  | DC   | P-O5'   | 6.28  | 1.66        | 1.59     | 3      | 2     |
| 1   | A     | 12  | DG   | C2-N2   | -6.25 | 1.28        | 1.34     | 6      | 2     |
| 2   | B     | 14  | DC   | C3'-C2' | 6.24  | 1.59        | 1.52     | 9      | 1     |
| 2   | B     | 18  | DG   | N7-C5   | 6.23  | 1.43        | 1.39     | 9      | 2     |
| 1   | A     | 5   | DA   | O3'-P   | 6.23  | 1.68        | 1.61     | 7      | 1     |
| 2   | B     | 16  | DC   | C2-O2   | -6.20 | 1.18        | 1.24     | 10     | 1     |
| 2   | B     | 18  | DG   | N9-C4   | -6.20 | 1.32        | 1.38     | 2      | 2     |
| 2   | B     | 14  | DC   | C4-N4   | -6.19 | 1.28        | 1.33     | 8      | 4     |
| 2   | B     | 21  | DC   | C2'-C1' | -6.19 | 1.46        | 1.52     | 6      | 4     |
| 1   | A     | 5   | DA   | C5'-C4' | 6.18  | 1.58        | 1.51     | 3      | 1     |
| 2   | B     | 17  | DG   | C8-N7   | -6.17 | 1.27        | 1.30     | 1      | 2     |
| 1   | A     | 6   | DG   | C6-N1   | -6.17 | 1.35        | 1.39     | 2      | 4     |
| 2   | B     | 15  | DC   | C5-C6   | 6.15  | 1.39        | 1.34     | 3      | 2     |
| 1   | A     | 3   | DA   | C5-C6   | 6.15  | 1.46        | 1.41     | 5      | 2     |
| 1   | A     | 2   | DC   | C3'-C2' | 6.13  | 1.59        | 1.52     | 3      | 1     |
| 2   | B     | 16  | DC   | C3'-C2' | 6.12  | 1.59        | 1.52     | 4      | 1     |
| 1   | A     | 9   | DC   | C5'-C4' | 6.12  | 1.58        | 1.51     | 7      | 1     |
| 1   | A     | 12  | DG   | C3'-O3' | 6.11  | 1.51        | 1.44     | 4      | 1     |
| 2   | B     | 20  | DC   | C2-O2   | -6.10 | 1.19        | 1.24     | 5      | 1     |
| 2   | B     | 22  | DT   | C2'-C1' | -6.10 | 1.46        | 1.52     | 6      | 1     |
| 1   | A     | 2   | DC   | C5'-C4' | 6.09  | 1.58        | 1.51     | 10     | 2     |
| 2   | B     | 20  | DC   | C2'-C1' | 6.07  | 1.58        | 1.52     | 8      | 4     |
| 2   | B     | 21  | DC   | C2-N3   | 6.06  | 1.40        | 1.35     | 2      | 1     |
| 1   | A     | 8   | DA   | P-O5'   | 6.06  | 1.65        | 1.59     | 6      | 1     |
| 2   | B     | 21  | DC   | N3-C4   | -6.06 | 1.29        | 1.33     | 4      | 2     |
| 2   | B     | 24  | DT   | C2'-C1' | 6.05  | 1.58        | 1.52     | 10     | 3     |
| 1   | A     | 8   | DA   | C4'-C3' | 6.04  | 1.59        | 1.53     | 5      | 1     |
| 1   | A     | 1   | DC   | C5'-C4' | 6.02  | 1.57        | 1.51     | 1      | 2     |
| 2   | B     | 23  | DT   | C2'-C1' | 6.01  | 1.58        | 1.52     | 2      | 2     |
| 2   | B     | 26  | DG   | C2-N2   | -6.00 | 1.28        | 1.34     | 2      | 2     |
| 2   | B     | 22  | DT   | N1-C6   | 6.00  | 1.42        | 1.38     | 2      | 3     |
| 1   | A     | 11  | DG   | N9-C8   | 5.99  | 1.42        | 1.37     | 8      | 2     |
| 1   | A     | 4   | DA   | C4'-O4' | -5.98 | 1.39        | 1.45     | 8      | 2     |
| 2   | B     | 18  | DG   | C2'-C1' | 5.97  | 1.58        | 1.52     | 5      | 3     |
| 2   | B     | 23  | DT   | C2-N3   | 5.97  | 1.42        | 1.37     | 1      | 2     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 2   | B     | 20  | DC   | C5'-C4' | 5.95  | 1.57        | 1.51     | 4      | 1     |
| 1   | A     | 2   | DC   | C2'-C1' | 5.95  | 1.58        | 1.52     | 5      | 1     |
| 2   | B     | 15  | DC   | C3'-C2' | 5.91  | 1.59        | 1.52     | 4      | 1     |
| 1   | A     | 8   | DA   | C4'-O4' | -5.90 | 1.39        | 1.45     | 10     | 1     |
| 2   | B     | 22  | DT   | C5'-C4' | 5.88  | 1.57        | 1.51     | 1      | 1     |
| 1   | A     | 12  | DG   | N1-C2   | -5.88 | 1.33        | 1.37     | 6      | 1     |
| 1   | A     | 13  | DG   | C3'-O3' | 5.87  | 1.51        | 1.44     | 9      | 1     |
| 1   | A     | 5   | DA   | C2-N3   | 5.86  | 1.38        | 1.33     | 7      | 2     |
| 2   | B     | 14  | DC   | C2-N3   | -5.86 | 1.31        | 1.35     | 10     | 1     |
| 2   | B     | 26  | DG   | C4'-C3' | 5.86  | 1.59        | 1.53     | 9      | 2     |
| 2   | B     | 19  | DT   | C4-O4   | 5.85  | 1.28        | 1.23     | 7      | 1     |
| 2   | B     | 23  | DT   | C4'-C3' | 5.85  | 1.59        | 1.53     | 3      | 1     |
| 2   | B     | 25  | DG   | N9-C4   | -5.82 | 1.33        | 1.38     | 7      | 2     |
| 1   | A     | 3   | DA   | N9-C8   | -5.82 | 1.33        | 1.37     | 9      | 1     |
| 1   | A     | 1   | DC   | C4-C5   | -5.81 | 1.38        | 1.43     | 9      | 1     |
| 2   | B     | 15  | DC   | N1-C2   | 5.79  | 1.46        | 1.40     | 7      | 1     |
| 2   | B     | 20  | DC   | C4'-C3' | 5.77  | 1.59        | 1.53     | 1      | 1     |
| 2   | B     | 22  | DT   | C3'-C2' | 5.76  | 1.59        | 1.52     | 9      | 1     |
| 1   | A     | 11  | DG   | O4'-C1' | 5.75  | 1.49        | 1.42     | 5      | 1     |
| 2   | B     | 17  | DG   | C5'-C4' | 5.74  | 1.57        | 1.51     | 4      | 1     |
| 1   | A     | 10  | DC   | C4'-O4' | -5.74 | 1.39        | 1.45     | 7      | 1     |
| 2   | B     | 15  | DC   | C2'-C1' | 5.73  | 1.58        | 1.52     | 2      | 1     |
| 2   | B     | 20  | DC   | N1-C2   | 5.72  | 1.45        | 1.40     | 2      | 1     |
| 2   | B     | 23  | DT   | C3'-C2' | 5.72  | 1.59        | 1.52     | 3      | 1     |
| 1   | A     | 12  | DG   | C3'-C2' | 5.71  | 1.59        | 1.52     | 9      | 1     |
| 2   | B     | 16  | DC   | C5-C6   | 5.71  | 1.39        | 1.34     | 2      | 1     |
| 2   | B     | 17  | DG   | N9-C4   | 5.71  | 1.42        | 1.38     | 7      | 2     |
| 2   | B     | 17  | DG   | C4'-O4' | -5.68 | 1.39        | 1.45     | 10     | 1     |
| 2   | B     | 25  | DG   | C2-N3   | 5.68  | 1.37        | 1.32     | 7      | 1     |
| 2   | B     | 24  | DT   | C4'-C3' | 5.67  | 1.59        | 1.53     | 7      | 2     |
| 2   | B     | 15  | DC   | C2-N3   | 5.66  | 1.40        | 1.35     | 7      | 1     |
| 1   | A     | 9   | DC   | N3-C4   | -5.65 | 1.29        | 1.33     | 9      | 2     |
| 1   | A     | 4   | DA   | C2-N3   | -5.63 | 1.28        | 1.33     | 7      | 1     |
| 2   | B     | 15  | DC   | N3-C4   | -5.63 | 1.30        | 1.33     | 6      | 1     |
| 2   | B     | 16  | DC   | N1-C2   | 5.58  | 1.45        | 1.40     | 5      | 2     |
| 2   | B     | 25  | DG   | C4'-O4' | -5.58 | 1.39        | 1.45     | 6      | 2     |
| 2   | B     | 25  | DG   | N9-C8   | 5.57  | 1.41        | 1.37     | 6      | 1     |
| 2   | B     | 23  | DT   | P-O5'   | -5.55 | 1.54        | 1.59     | 7      | 2     |
| 2   | B     | 26  | DG   | N1-C2   | -5.55 | 1.33        | 1.37     | 9      | 1     |
| 1   | A     | 9   | DC   | O4'-C1' | -5.54 | 1.35        | 1.42     | 6      | 1     |
| 2   | B     | 18  | DG   | C5-C6   | 5.54  | 1.47        | 1.42     | 7      | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 4   | DA   | C4'-C3' | 5.54  | 1.58        | 1.53     | 8      | 1     |
| 2   | B     | 17  | DG   | C6-N1   | -5.53 | 1.35        | 1.39     | 6      | 1     |
| 2   | B     | 25  | DG   | O4'-C1' | 5.50  | 1.48        | 1.42     | 3      | 1     |
| 2   | B     | 25  | DG   | C5-C4   | 5.50  | 1.42        | 1.38     | 9      | 2     |
| 1   | A     | 6   | DG   | N1-C2   | -5.49 | 1.33        | 1.37     | 5      | 1     |
| 2   | B     | 15  | DC   | O4'-C1' | -5.48 | 1.35        | 1.42     | 10     | 1     |
| 1   | A     | 5   | DA   | C4'-C3' | 5.48  | 1.58        | 1.53     | 6      | 1     |
| 2   | B     | 20  | DC   | C4-C5   | -5.47 | 1.38        | 1.43     | 1      | 2     |
| 1   | A     | 1   | DC   | C2'-C1' | -5.47 | 1.46        | 1.52     | 2      | 2     |
| 1   | A     | 10  | DC   | C5-C6   | 5.46  | 1.38        | 1.34     | 3      | 3     |
| 1   | A     | 11  | DG   | C2-N3   | 5.45  | 1.37        | 1.32     | 6      | 1     |
| 1   | A     | 11  | DG   | C3'-O3' | -5.44 | 1.36        | 1.44     | 5      | 1     |
| 2   | B     | 14  | DC   | C4-C5   | -5.44 | 1.38        | 1.43     | 2      | 1     |
| 2   | B     | 14  | DC   | C5-C6   | 5.43  | 1.38        | 1.34     | 2      | 1     |
| 1   | A     | 8   | DA   | C3'-O3' | -5.42 | 1.36        | 1.44     | 5      | 2     |
| 1   | A     | 1   | DC   | C4'-C3' | 5.41  | 1.58        | 1.53     | 1      | 1     |
| 2   | B     | 19  | DT   | C2'-C1' | 5.39  | 1.57        | 1.52     | 10     | 1     |
| 1   | A     | 2   | DC   | C2-O2   | -5.37 | 1.19        | 1.24     | 1      | 1     |
| 1   | A     | 9   | DC   | O3'-P   | 5.34  | 1.67        | 1.61     | 6      | 1     |
| 1   | A     | 3   | DA   | C4'-C3' | 5.34  | 1.58        | 1.53     | 1      | 1     |
| 2   | B     | 15  | DC   | C1'-N1  | 5.33  | 1.56        | 1.49     | 2      | 1     |
| 1   | A     | 1   | DC   | C3'-C2' | 5.33  | 1.58        | 1.52     | 4      | 1     |
| 1   | A     | 6   | DG   | C8-N7   | 5.32  | 1.34        | 1.30     | 5      | 1     |
| 2   | B     | 20  | DC   | O4'-C1' | 5.30  | 1.48        | 1.42     | 3      | 1     |
| 1   | A     | 13  | DG   | C5-C4   | 5.30  | 1.42        | 1.38     | 4      | 1     |
| 2   | B     | 17  | DG   | C2'-C1' | 5.30  | 1.57        | 1.52     | 2      | 2     |
| 1   | A     | 11  | DG   | N1-C2   | 5.29  | 1.42        | 1.37     | 3      | 1     |
| 2   | B     | 17  | DG   | C3'-C2' | 5.28  | 1.58        | 1.52     | 10     | 1     |
| 2   | B     | 22  | DT   | N3-C4   | -5.28 | 1.34        | 1.38     | 6      | 1     |
| 2   | B     | 24  | DT   | C5'-C4' | 5.27  | 1.57        | 1.51     | 4      | 1     |
| 1   | A     | 13  | DG   | C2'-C1' | -5.27 | 1.47        | 1.52     | 10     | 1     |
| 2   | B     | 18  | DG   | C8-N7   | 5.26  | 1.34        | 1.30     | 3      | 2     |
| 1   | A     | 9   | DC   | C4'-C3' | -5.24 | 1.47        | 1.52     | 6      | 1     |
| 1   | A     | 12  | DG   | C1'-N9  | 5.24  | 1.56        | 1.49     | 8      | 1     |
| 2   | B     | 19  | DT   | O3'-P   | 5.19  | 1.67        | 1.61     | 7      | 1     |
| 2   | B     | 18  | DG   | O4'-C1' | -5.17 | 1.36        | 1.42     | 6      | 1     |
| 1   | A     | 4   | DA   | C3'-O3' | -5.17 | 1.37        | 1.44     | 7      | 1     |
| 2   | B     | 19  | DT   | C3'-C2' | 5.14  | 1.58        | 1.52     | 3      | 1     |
| 2   | B     | 22  | DT   | C4-C5   | 5.13  | 1.49        | 1.45     | 5      | 1     |
| 2   | B     | 18  | DG   | C2-N3   | -5.13 | 1.28        | 1.32     | 7      | 1     |
| 2   | B     | 15  | DC   | C3'-O3' | -5.12 | 1.37        | 1.44     | 6      | 1     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 2   | B     | 19  | DT   | N1-C6 | 5.11  | 1.41        | 1.38     | 3      | 1     |
| 2   | B     | 17  | DG   | O3'-P | 5.10  | 1.67        | 1.61     | 2      | 1     |
| 1   | A     | 2   | DC   | O3'-P | -5.09 | 1.55        | 1.61     | 5      | 1     |
| 1   | A     | 2   | DC   | C5-C6 | -5.08 | 1.30        | 1.34     | 8      | 1     |
| 2   | B     | 24  | DT   | C2-N3 | -5.06 | 1.33        | 1.37     | 8      | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
|     |       |     |      |             |        |             |          | Worst  | Total |
| 1   | A     | 1   | DC   | N3-C4-C5    | 19.64  | 129.76      | 121.90   | 10     | 5     |
| 2   | B     | 23  | DT   | N3-C2-O2    | -19.49 | 110.60      | 122.30   | 10     | 6     |
| 2   | B     | 26  | DG   | O4'-C1'-N9  | 18.59  | 121.02      | 108.00   | 9      | 6     |
| 1   | A     | 5   | DA   | N1-C6-N6    | -18.58 | 107.45      | 118.60   | 5      | 10    |
| 1   | A     | 12  | DG   | O4'-C1'-N9  | 18.50  | 120.95      | 108.00   | 6      | 7     |
| 1   | A     | 11  | DG   | C2-N3-C4    | 18.48  | 121.14      | 111.90   | 7      | 4     |
| 1   | A     | 11  | DG   | C8-N9-C4    | -18.23 | 99.11       | 106.40   | 8      | 3     |
| 1   | A     | 10  | DC   | O4'-C1'-N1  | 17.94  | 120.56      | 108.00   | 5      | 5     |
| 1   | A     | 3   | DA   | N1-C6-N6    | -17.94 | 107.84      | 118.60   | 4      | 8     |
| 2   | B     | 15  | DC   | N3-C2-O2    | -17.42 | 109.71      | 121.90   | 7      | 11    |
| 2   | B     | 22  | DT   | N3-C2-O2    | -17.35 | 111.89      | 122.30   | 5      | 7     |
| 1   | A     | 11  | DG   | N3-C4-C5    | -17.07 | 120.06      | 128.60   | 7      | 5     |
| 2   | B     | 25  | DG   | N9-C4-C5    | 16.58  | 112.03      | 105.40   | 7      | 3     |
| 1   | A     | 3   | DA   | C5-C6-N1    | 16.57  | 125.98      | 117.70   | 10     | 6     |
| 1   | A     | 2   | DC   | C5-C6-N1    | -16.52 | 112.74      | 121.00   | 4      | 4     |
| 2   | B     | 18  | DG   | O4'-C1'-N9  | 16.36  | 119.45      | 108.00   | 1      | 6     |
| 1   | A     | 6   | DG   | C2-N3-C4    | 16.23  | 120.02      | 111.90   | 1      | 3     |
| 1   | A     | 9   | DC   | N3-C2-O2    | -16.21 | 110.55      | 121.90   | 5      | 9     |
| 1   | A     | 5   | DA   | C5-C6-N1    | 16.20  | 125.80      | 117.70   | 5      | 9     |
| 1   | A     | 2   | DC   | N3-C4-C5    | 16.16  | 128.36      | 121.90   | 5      | 6     |
| 2   | B     | 22  | DT   | O4'-C1'-N1  | 16.12  | 119.28      | 108.00   | 8      | 7     |
| 2   | B     | 19  | DT   | O4'-C1'-N1  | 16.05  | 119.24      | 108.00   | 6      | 4     |
| 2   | B     | 21  | DC   | N1-C2-O2    | 16.04  | 128.52      | 118.90   | 2      | 5     |
| 2   | B     | 20  | DC   | N1-C2-O2    | 15.89  | 128.43      | 118.90   | 7      | 8     |
| 1   | A     | 8   | DA   | N1-C6-N6    | -15.74 | 109.16      | 118.60   | 9      | 11    |
| 1   | A     | 6   | DG   | O4'-C1'-N9  | 15.64  | 118.95      | 108.00   | 7      | 8     |
| 1   | A     | 4   | DA   | N1-C6-N6    | -15.55 | 109.27      | 118.60   | 8      | 10    |
| 1   | A     | 2   | DC   | O4'-C4'-C3' | 15.47  | 115.28      | 106.00   | 7      | 3     |
| 2   | B     | 21  | DC   | N3-C2-O2    | -15.29 | 111.20      | 121.90   | 10     | 8     |
| 2   | B     | 22  | DT   | C6-C5-C7    | -15.03 | 113.89      | 122.90   | 1      | 6     |
| 2   | B     | 19  | DT   | N3-C2-O2    | -14.97 | 113.31      | 122.30   | 5      | 7     |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
|     |       |     |      |            |        |             |          | Worst  | Total |
| 1   | A     | 2   | DC   | N3-C2-O2   | -14.91 | 111.46      | 121.90   | 10     | 10    |
| 2   | B     | 16  | DC   | O4'-C1'-N1 | 14.80  | 118.36      | 108.00   | 10     | 6     |
| 2   | B     | 17  | DG   | N3-C2-N2   | -14.77 | 109.56      | 119.90   | 5      | 6     |
| 2   | B     | 20  | DC   | N3-C2-O2   | -14.68 | 111.63      | 121.90   | 5      | 9     |
| 2   | B     | 19  | DT   | C6-C5-C7   | -14.66 | 114.10      | 122.90   | 5      | 7     |
| 1   | A     | 8   | DA   | C5-C6-N1   | 14.57  | 124.98      | 117.70   | 6      | 10    |
| 2   | B     | 18  | DG   | N1-C6-O6   | -14.53 | 111.18      | 119.90   | 7      | 5     |
| 2   | B     | 15  | DC   | N1-C2-O2   | 14.44  | 127.57      | 118.90   | 7      | 6     |
| 2   | B     | 20  | DC   | N3-C4-C5   | 14.43  | 127.67      | 121.90   | 2      | 7     |
| 1   | A     | 11  | DG   | N1-C6-O6   | -14.41 | 111.25      | 119.90   | 3      | 6     |
| 2   | B     | 19  | DT   | N1-C2-N3   | 14.35  | 123.21      | 114.60   | 9      | 3     |
| 1   | A     | 8   | DA   | C4-C5-C6   | -14.29 | 109.86      | 117.00   | 7      | 10    |
| 2   | B     | 22  | DT   | N1-C2-N3   | 14.29  | 123.17      | 114.60   | 5      | 4     |
| 2   | B     | 19  | DT   | C5-C6-N1   | -14.27 | 115.14      | 123.70   | 8      | 5     |
| 2   | B     | 23  | DT   | O4'-C1'-N1 | 13.91  | 117.74      | 108.00   | 1      | 5     |
| 2   | B     | 15  | DC   | C6-N1-C2   | -13.89 | 114.74      | 120.30   | 1      | 4     |
| 2   | B     | 18  | DG   | C5-C6-O6   | 13.73  | 136.84      | 128.60   | 7      | 2     |
| 2   | B     | 14  | DC   | C6-N1-C2   | -13.71 | 114.81      | 120.30   | 7      | 1     |
| 2   | B     | 16  | DC   | N1-C2-O2   | 13.70  | 127.12      | 118.90   | 7      | 5     |
| 2   | B     | 25  | DG   | O4'-C1'-N9 | 13.68  | 117.58      | 108.00   | 1      | 6     |
| 1   | A     | 4   | DA   | N1-C2-N3   | -13.59 | 122.50      | 129.30   | 3      | 3     |
| 1   | A     | 12  | DG   | C2-N3-C4   | 13.57  | 118.69      | 111.90   | 4      | 6     |
| 1   | A     | 1   | DC   | N1-C2-O2   | 13.54  | 127.02      | 118.90   | 8      | 6     |
| 1   | A     | 13  | DG   | N7-C8-N9   | 13.51  | 119.86      | 113.10   | 1      | 2     |
| 1   | A     | 13  | DG   | C5-N7-C8   | -13.51 | 97.55       | 104.30   | 1      | 1     |
| 2   | B     | 23  | DT   | C6-C5-C7   | -13.50 | 114.80      | 122.90   | 3      | 8     |
| 2   | B     | 26  | DG   | N1-C6-O6   | -13.47 | 111.82      | 119.90   | 4      | 4     |
| 2   | B     | 25  | DG   | N3-C4-C5   | -13.44 | 121.88      | 128.60   | 2      | 3     |
| 2   | B     | 23  | DT   | N3-C4-O4   | 13.42  | 127.95      | 119.90   | 9      | 3     |
| 2   | B     | 20  | DC   | O4'-C1'-N1 | 13.39  | 117.37      | 108.00   | 7      | 6     |
| 1   | A     | 10  | DC   | N3-C4-C5   | 13.38  | 127.25      | 121.90   | 9      | 4     |
| 2   | B     | 18  | DG   | N3-C2-N2   | -13.35 | 110.55      | 119.90   | 3      | 5     |
| 2   | B     | 14  | DC   | N3-C4-C5   | 13.30  | 127.22      | 121.90   | 3      | 5     |
| 1   | A     | 4   | DA   | O4'-C1'-N9 | 13.30  | 117.31      | 108.00   | 6      | 7     |
| 2   | B     | 15  | DC   | O4'-C1'-N1 | 13.29  | 117.30      | 108.00   | 9      | 6     |
| 2   | B     | 17  | DG   | O4'-C1'-N9 | 13.21  | 117.25      | 108.00   | 9      | 6     |
| 2   | B     | 19  | DT   | C6-N1-C2   | -13.21 | 114.70      | 121.30   | 9      | 4     |
| 2   | B     | 25  | DG   | N1-C2-N3   | 13.16  | 131.80      | 123.90   | 6      | 5     |
| 2   | B     | 20  | DC   | N3-C4-N4   | -13.14 | 108.80      | 118.00   | 10     | 6     |
| 1   | A     | 12  | DG   | C4-C5-N7   | -13.14 | 105.55      | 110.80   | 2      | 7     |
| 2   | B     | 25  | DG   | C6-N1-C2   | -13.06 | 117.26      | 125.10   | 6      | 4     |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
|     |       |     |      |             |        |             |          | Worst  | Total |
| 2   | B     | 15  | DC   | O4'-C1'-C2' | -13.02 | 95.49       | 105.90   | 3      | 3     |
| 2   | B     | 25  | DG   | N1-C6-O6    | -12.98 | 112.11      | 119.90   | 2      | 5     |
| 1   | A     | 10  | DC   | C6-N1-C2    | -12.92 | 115.13      | 120.30   | 4      | 5     |
| 2   | B     | 18  | DG   | O4'-C4'-C3' | 12.90  | 113.74      | 106.00   | 8      | 4     |
| 1   | A     | 2   | DC   | O4'-C1'-N1  | 12.86  | 117.00      | 108.00   | 2      | 5     |
| 2   | B     | 15  | DC   | N3-C4-C5    | -12.77 | 116.79      | 121.90   | 3      | 5     |
| 2   | B     | 14  | DC   | N3-C2-O2    | -12.74 | 112.98      | 121.90   | 1      | 9     |
| 1   | A     | 9   | DC   | C5-C6-N1    | -12.73 | 114.63      | 121.00   | 10     | 2     |
| 1   | A     | 12  | DG   | N9-C4-C5    | 12.71  | 110.49      | 105.40   | 4      | 6     |
| 2   | B     | 18  | DG   | N9-C4-C5    | 12.70  | 110.48      | 105.40   | 3      | 2     |
| 1   | A     | 12  | DG   | N3-C4-C5    | -12.65 | 122.28      | 128.60   | 4      | 3     |
| 1   | A     | 8   | DA   | N9-C4-C5    | -12.65 | 100.74      | 105.80   | 7      | 3     |
| 2   | B     | 24  | DT   | C6-C5-C7    | -12.59 | 115.34      | 122.90   | 3      | 8     |
| 1   | A     | 8   | DA   | O4'-C1'-N9  | 12.59  | 116.81      | 108.00   | 4      | 3     |
| 1   | A     | 5   | DA   | C4-C5-C6    | -12.58 | 110.71      | 117.00   | 9      | 9     |
| 1   | A     | 4   | DA   | C4-C5-C6    | -12.55 | 110.72      | 117.00   | 1      | 7     |
| 2   | B     | 25  | DG   | C8-N9-C4    | -12.55 | 101.38      | 106.40   | 6      | 5     |
| 2   | B     | 25  | DG   | C4-C5-N7    | -12.54 | 105.78      | 110.80   | 7      | 2     |
| 1   | A     | 3   | DA   | N1-C2-N3    | -12.53 | 123.03      | 129.30   | 8      | 5     |
| 1   | A     | 9   | DC   | N3-C4-C5    | 12.50  | 126.90      | 121.90   | 7      | 3     |
| 2   | B     | 14  | DC   | N1-C2-O2    | 12.49  | 126.39      | 118.90   | 1      | 5     |
| 1   | A     | 12  | DG   | C6-C5-N7    | 12.48  | 137.89      | 130.40   | 2      | 5     |
| 2   | B     | 24  | DT   | N3-C2-O2    | -12.45 | 114.83      | 122.30   | 3      | 6     |
| 2   | B     | 23  | DT   | O4'-C4'-C3' | 12.45  | 113.47      | 106.00   | 8      | 5     |
| 1   | A     | 5   | DA   | N1-C2-N3    | -12.41 | 123.09      | 129.30   | 4      | 7     |
| 2   | B     | 15  | DC   | N3-C4-N4    | -12.41 | 109.31      | 118.00   | 5      | 5     |
| 2   | B     | 21  | DC   | N3-C4-C5    | 12.38  | 126.85      | 121.90   | 1      | 5     |
| 2   | B     | 19  | DT   | C4-C5-C7    | 12.38  | 126.43      | 119.00   | 5      | 2     |
| 1   | A     | 8   | DA   | O4'-C4'-C3' | 12.35  | 113.41      | 106.00   | 1      | 5     |
| 1   | A     | 13  | DG   | O4'-C1'-N9  | 12.33  | 116.63      | 108.00   | 10     | 5     |
| 1   | A     | 10  | DC   | N1-C2-O2    | 12.31  | 126.28      | 118.90   | 3      | 5     |
| 1   | A     | 12  | DG   | N1-C6-O6    | -12.28 | 112.53      | 119.90   | 7      | 6     |
| 1   | A     | 12  | DG   | O4'-C4'-C3' | 12.24  | 113.35      | 106.00   | 1      | 4     |
| 1   | A     | 5   | DA   | O4'-C4'-C3' | 12.24  | 113.34      | 106.00   | 1      | 6     |
| 1   | A     | 3   | DA   | O4'-C1'-C2' | -12.24 | 96.11       | 105.90   | 7      | 3     |
| 1   | A     | 9   | DC   | N1-C2-O2    | 12.24  | 126.24      | 118.90   | 9      | 8     |
| 2   | B     | 17  | DG   | C5-C6-N1    | 12.23  | 117.61      | 111.50   | 8      | 2     |
| 1   | A     | 1   | DC   | N3-C4-N4    | -12.20 | 109.46      | 118.00   | 7      | 4     |
| 2   | B     | 17  | DG   | N1-C6-O6    | -12.19 | 112.59      | 119.90   | 10     | 4     |
| 1   | A     | 11  | DG   | N7-C8-N9    | 12.18  | 119.19      | 113.10   | 8      | 2     |
| 1   | A     | 9   | DC   | C2-N3-C4    | -12.14 | 113.83      | 119.90   | 7      | 5     |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
|     |       |     |      |             |        |             |          | Worst  | Total |
| 1   | A     | 8   | DA   | C6-N1-C2    | -12.12 | 111.33      | 118.60   | 9      | 2     |
| 1   | A     | 9   | DC   | N3-C4-N4    | -12.07 | 109.55      | 118.00   | 3      | 4     |
| 1   | A     | 10  | DC   | O4'-C4'-C3' | 12.01  | 113.21      | 106.00   | 5      | 5     |
| 2   | B     | 24  | DT   | N3-C4-O4    | -11.86 | 112.78      | 119.90   | 5      | 4     |
| 2   | B     | 24  | DT   | N1-C2-N3    | 11.83  | 121.70      | 114.60   | 7      | 6     |
| 2   | B     | 14  | DC   | C5-C6-N1    | -11.82 | 115.09      | 121.00   | 8      | 3     |
| 1   | A     | 11  | DG   | C5-C6-N1    | 11.81  | 117.41      | 111.50   | 4      | 7     |
| 2   | B     | 15  | DC   | C2-N3-C4    | -11.79 | 114.00      | 119.90   | 10     | 5     |
| 2   | B     | 14  | DC   | C5-C4-N4    | 11.71  | 128.40      | 120.20   | 6      | 3     |
| 2   | B     | 22  | DT   | C4-C5-C7    | 11.70  | 126.02      | 119.00   | 1      | 3     |
| 1   | A     | 9   | DC   | C4-C5-C6    | 11.67  | 123.24      | 117.40   | 10     | 2     |
| 2   | B     | 24  | DT   | O4'-C1'-N1  | 11.61  | 116.13      | 108.00   | 9      | 6     |
| 1   | A     | 6   | DG   | N3-C2-N2    | -11.58 | 111.80      | 119.90   | 5      | 5     |
| 1   | A     | 6   | DG   | N1-C6-O6    | -11.54 | 112.97      | 119.90   | 5      | 6     |
| 1   | A     | 8   | DA   | C6-C5-N7    | 11.53  | 140.37      | 132.30   | 10     | 6     |
| 1   | A     | 8   | DA   | C2-N3-C4    | 11.51  | 116.36      | 110.60   | 5      | 5     |
| 1   | A     | 13  | DG   | C6-N1-C2    | -11.46 | 118.22      | 125.10   | 10     | 3     |
| 2   | B     | 25  | DG   | O4'-C4'-C3' | 11.44  | 112.86      | 106.00   | 9      | 4     |
| 2   | B     | 20  | DC   | C2-N3-C4    | -11.40 | 114.20      | 119.90   | 5      | 4     |
| 1   | A     | 1   | DC   | C6-N1-C2    | 11.39  | 124.86      | 120.30   | 8      | 3     |
| 2   | B     | 21  | DC   | C2-N3-C4    | -11.34 | 114.23      | 119.90   | 10     | 3     |
| 1   | A     | 6   | DG   | N1-C2-N3    | 11.34  | 130.70      | 123.90   | 4      | 3     |
| 1   | A     | 2   | DC   | N3-C4-N4    | -11.31 | 110.08      | 118.00   | 9      | 7     |
| 1   | A     | 11  | DG   | O4'-C4'-C3' | 11.31  | 112.78      | 106.00   | 9      | 5     |
| 2   | B     | 25  | DG   | C5-N7-C8    | -11.29 | 98.66       | 104.30   | 3      | 6     |
| 1   | A     | 2   | DC   | C2-N3-C4    | -11.24 | 114.28      | 119.90   | 1      | 5     |
| 2   | B     | 25  | DG   | N3-C2-N2    | -11.23 | 112.04      | 119.90   | 3      | 4     |
| 1   | A     | 1   | DC   | N3-C2-O2    | -11.21 | 114.05      | 121.90   | 4      | 10    |
| 1   | A     | 11  | DG   | C6-C5-N7    | 11.20  | 137.12      | 130.40   | 3      | 4     |
| 2   | B     | 22  | DT   | O4'-C4'-C3' | 11.19  | 112.71      | 106.00   | 7      | 5     |
| 2   | B     | 15  | DC   | C5-C4-N4    | 11.18  | 128.03      | 120.20   | 5      | 2     |
| 1   | A     | 10  | DC   | N3-C2-O2    | -11.16 | 114.09      | 121.90   | 3      | 8     |
| 1   | A     | 2   | DC   | C4-C5-C6    | -11.15 | 111.82      | 117.40   | 5      | 6     |
| 1   | A     | 6   | DG   | N9-C4-C5    | 11.15  | 109.86      | 105.40   | 1      | 3     |
| 2   | B     | 20  | DC   | O4'-C4'-C3' | 11.13  | 112.68      | 106.00   | 1      | 4     |
| 2   | B     | 17  | DG   | C6-N1-C2    | -11.12 | 118.43      | 125.10   | 10     | 4     |
| 1   | A     | 4   | DA   | C2-N3-C4    | 11.09  | 116.15      | 110.60   | 8      | 6     |
| 2   | B     | 16  | DC   | N3-C4-C5    | 11.09  | 126.33      | 121.90   | 6      | 6     |
| 1   | A     | 13  | DG   | N1-C6-O6    | -11.08 | 113.25      | 119.90   | 10     | 3     |
| 1   | A     | 6   | DG   | C4-C5-N7    | 11.06  | 115.22      | 110.80   | 5      | 6     |
| 1   | A     | 2   | DC   | N1-C2-O2    | 11.06  | 125.53      | 118.90   | 10     | 8     |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
|     |       |     |      |             |        |             |          | Worst  | Total |
| 1   | A     | 4   | DA   | C5-C6-N1    | 11.05  | 123.23      | 117.70   | 4      | 9     |
| 2   | B     | 26  | DG   | N3-C4-C5    | -11.05 | 123.07      | 128.60   | 7      | 4     |
| 1   | A     | 5   | DA   | C6-N1-C2    | -11.03 | 111.98      | 118.60   | 5      | 3     |
| 1   | A     | 6   | DG   | N3-C4-C5    | -11.01 | 123.09      | 128.60   | 1      | 6     |
| 1   | A     | 13  | DG   | O4'-C4'-C3' | 11.01  | 112.61      | 106.00   | 3      | 6     |
| 2   | B     | 16  | DC   | C6-N1-C2    | -11.01 | 115.90      | 120.30   | 3      | 2     |
| 2   | B     | 25  | DG   | C6-C5-N7    | 10.97  | 136.98      | 130.40   | 8      | 3     |
| 1   | A     | 9   | DC   | C5-C4-N4    | 10.94  | 127.86      | 120.20   | 10     | 3     |
| 2   | B     | 21  | DC   | O4'-C1'-N1  | 10.94  | 115.66      | 108.00   | 9      | 9     |
| 1   | A     | 1   | DC   | O4'-C1'-N1  | 10.89  | 115.62      | 108.00   | 7      | 7     |
| 2   | B     | 21  | DC   | N1-C2-N3    | 10.88  | 126.81      | 119.20   | 10     | 3     |
| 2   | B     | 26  | DG   | C5-C6-N1    | 10.87  | 116.94      | 111.50   | 4      | 2     |
| 1   | A     | 10  | DC   | N3-C4-N4    | -10.84 | 110.42      | 118.00   | 9      | 4     |
| 2   | B     | 18  | DG   | C4-C5-N7    | -10.78 | 106.49      | 110.80   | 3      | 4     |
| 2   | B     | 17  | DG   | C2-N3-C4    | -10.78 | 106.51      | 111.90   | 1      | 5     |
| 2   | B     | 16  | DC   | C2-N3-C4    | -10.77 | 114.52      | 119.90   | 9      | 4     |
| 1   | A     | 13  | DG   | N3-C2-N2    | -10.73 | 112.39      | 119.90   | 9      | 6     |
| 2   | B     | 23  | DT   | C5-C4-O4    | -10.71 | 117.41      | 124.90   | 9      | 4     |
| 1   | A     | 12  | DG   | C8-N9-C4    | -10.66 | 102.14      | 106.40   | 4      | 3     |
| 2   | B     | 23  | DT   | C4-C5-C6    | 10.65  | 124.39      | 118.00   | 6      | 4     |
| 2   | B     | 17  | DG   | N1-C2-N2    | 10.65  | 125.78      | 116.20   | 4      | 4     |
| 2   | B     | 25  | DG   | C2-N3-C4    | 10.62  | 117.21      | 111.90   | 2      | 2     |
| 1   | A     | 9   | DC   | O4'-C1'-N1  | 10.60  | 115.42      | 108.00   | 7      | 5     |
| 2   | B     | 20  | DC   | C6-N1-C2    | -10.56 | 116.08      | 120.30   | 1      | 5     |
| 2   | B     | 19  | DT   | C5-C4-O4    | 10.55  | 132.29      | 124.90   | 3      | 1     |
| 2   | B     | 24  | DT   | C6-N1-C2    | -10.55 | 116.03      | 121.30   | 2      | 5     |
| 2   | B     | 22  | DT   | N3-C4-O4    | -10.49 | 113.61      | 119.90   | 7      | 4     |
| 2   | B     | 18  | DG   | C6-N1-C2    | -10.40 | 118.86      | 125.10   | 3      | 1     |
| 2   | B     | 16  | DC   | N3-C2-O2    | -10.34 | 114.66      | 121.90   | 3      | 9     |
| 1   | A     | 8   | DA   | C4-C5-N7    | -10.29 | 105.55      | 110.70   | 10     | 4     |
| 2   | B     | 19  | DT   | C4-C5-C6    | 10.23  | 124.14      | 118.00   | 3      | 3     |
| 1   | A     | 13  | DG   | C4-C5-N7    | 10.21  | 114.89      | 110.80   | 1      | 2     |
| 1   | A     | 11  | DG   | O4'-C1'-N9  | 10.18  | 115.12      | 108.00   | 8      | 3     |
| 2   | B     | 21  | DC   | O4'-C4'-C3' | -10.18 | 99.89       | 106.00   | 6      | 2     |
| 1   | A     | 1   | DC   | C2-N3-C4    | -10.14 | 114.83      | 119.90   | 1      | 6     |
| 2   | B     | 17  | DG   | C5-N7-C8    | -10.13 | 99.23       | 104.30   | 9      | 1     |
| 2   | B     | 14  | DC   | N3-C4-N4    | -10.12 | 110.91      | 118.00   | 3      | 5     |
| 2   | B     | 14  | DC   | O4'-C4'-C3' | 10.12  | 112.07      | 106.00   | 7      | 6     |
| 2   | B     | 22  | DT   | C2-N3-C4    | -10.07 | 121.16      | 127.20   | 5      | 2     |
| 1   | A     | 13  | DG   | N1-C2-N3    | 10.06  | 129.94      | 123.90   | 10     | 2     |
| 1   | A     | 1   | DC   | C4-C5-C6    | -10.04 | 112.38      | 117.40   | 10     | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
|     |       |     |      |             |        |             |          | Worst  | Total |
| 2   | B     | 19  | DT   | C2-N3-C4    | -10.01 | 121.20      | 127.20   | 7      | 3     |
| 1   | A     | 13  | DG   | C5-C6-N1    | 9.98   | 116.49      | 111.50   | 1      | 5     |
| 2   | B     | 17  | DG   | N1-C2-N3    | 9.95   | 129.87      | 123.90   | 10     | 6     |
| 2   | B     | 26  | DG   | N7-C8-N9    | 9.94   | 118.07      | 113.10   | 6      | 4     |
| 1   | A     | 11  | DG   | C4-C5-N7    | -9.93  | 106.83      | 110.80   | 2      | 5     |
| 2   | B     | 25  | DG   | N7-C8-N9    | 9.91   | 118.06      | 113.10   | 10     | 7     |
| 2   | B     | 22  | DT   | C4'-C3'-C2' | 9.88   | 111.99      | 103.10   | 10     | 2     |
| 1   | A     | 4   | DA   | O4'-C4'-C3' | 9.85   | 111.91      | 106.00   | 9      | 5     |
| 2   | B     | 21  | DC   | C4-C5-C6    | -9.83  | 112.48      | 117.40   | 1      | 2     |
| 2   | B     | 15  | DC   | C4-C5-C6    | 9.78   | 122.29      | 117.40   | 3      | 3     |
| 2   | B     | 17  | DG   | O4'-C4'-C3' | 9.71   | 111.83      | 106.00   | 1      | 3     |
| 2   | B     | 15  | DC   | N1-C2-N3    | 9.71   | 125.99      | 119.20   | 10     | 2     |
| 1   | A     | 12  | DG   | C5-C6-O6    | -9.61  | 122.83      | 128.60   | 6      | 4     |
| 2   | B     | 26  | DG   | N3-C4-N9    | 9.57   | 131.74      | 126.00   | 7      | 2     |
| 1   | A     | 5   | DA   | C4'-C3'-C2' | -9.56  | 94.50       | 103.10   | 1      | 2     |
| 2   | B     | 23  | DT   | C5-C6-N1    | -9.54  | 117.98      | 123.70   | 10     | 4     |
| 2   | B     | 17  | DG   | N7-C8-N9    | 9.53   | 117.86      | 113.10   | 9      | 1     |
| 1   | A     | 6   | DG   | C6-N1-C2    | -9.52  | 119.39      | 125.10   | 3      | 3     |
| 2   | B     | 14  | DC   | C2-N3-C4    | -9.48  | 115.16      | 119.90   | 9      | 3     |
| 2   | B     | 18  | DG   | P-O3'-C3'   | 9.45   | 131.04      | 119.70   | 8      | 2     |
| 2   | B     | 26  | DG   | N3-C2-N2    | -9.44  | 113.29      | 119.90   | 8      | 5     |
| 1   | A     | 1   | DC   | O4'-C4'-C3' | 9.43   | 111.66      | 106.00   | 9      | 1     |
| 1   | A     | 6   | DG   | N7-C8-N9    | 9.41   | 117.81      | 113.10   | 7      | 1     |
| 2   | B     | 16  | DC   | C4-C5-C6    | 9.40   | 122.10      | 117.40   | 3      | 3     |
| 1   | A     | 1   | DC   | N1-C2-N3    | 9.36   | 125.75      | 119.20   | 1      | 3     |
| 1   | A     | 2   | DC   | C6-N1-C2    | -9.36  | 116.56      | 120.30   | 1      | 2     |
| 2   | B     | 25  | DG   | C5-C6-N1    | 9.33   | 116.17      | 111.50   | 9      | 4     |
| 1   | A     | 13  | DG   | N9-C4-C5    | 9.31   | 109.13      | 105.40   | 6      | 3     |
| 1   | A     | 8   | DA   | C8-N9-C4    | -9.26  | 102.09      | 105.80   | 4      | 6     |
| 2   | B     | 22  | DT   | C5-C6-N1    | -9.25  | 118.15      | 123.70   | 2      | 5     |
| 2   | B     | 17  | DG   | N3-C4-N9    | 9.23   | 131.54      | 126.00   | 4      | 1     |
| 2   | B     | 16  | DC   | N3-C4-N4    | -9.23  | 111.54      | 118.00   | 6      | 2     |
| 2   | B     | 26  | DG   | C1'-O4'-C4' | -9.22  | 100.88      | 110.10   | 1      | 2     |
| 2   | B     | 20  | DC   | C4'-C3'-C2' | -9.20  | 94.82       | 103.10   | 1      | 1     |
| 2   | B     | 15  | DC   | C5-C6-N1    | 9.14   | 125.57      | 121.00   | 1      | 4     |
| 2   | B     | 19  | DT   | C4'-C3'-C2' | -9.12  | 94.89       | 103.10   | 8      | 1     |
| 1   | A     | 13  | DG   | C8-N9-C4    | -9.12  | 102.75      | 106.40   | 1      | 1     |
| 1   | A     | 11  | DG   | C6-N1-C2    | -9.11  | 119.63      | 125.10   | 4      | 3     |
| 1   | A     | 12  | DG   | C5-C6-N1    | 9.07   | 116.04      | 111.50   | 8      | 5     |
| 2   | B     | 26  | DG   | O4'-C1'-C2' | -9.00  | 98.70       | 105.90   | 6      | 2     |
| 1   | A     | 3   | DA   | C4-C5-C6    | -9.00  | 112.50      | 117.00   | 10     | 8     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 2   | B     | 24  | DT   | O4'-C4'-C3' | 8.98  | 111.39      | 106.00   | 7      | 4     |
| 1   | A     | 3   | DA   | C5-N7-C8    | -8.97 | 99.41       | 103.90   | 10     | 4     |
| 1   | A     | 4   | DA   | C6-C5-N7    | 8.94  | 138.56      | 132.30   | 3      | 4     |
| 1   | A     | 12  | DG   | C4-C5-C6    | -8.92 | 113.45      | 118.80   | 1      | 3     |
| 1   | A     | 10  | DC   | C2-N3-C4    | -8.90 | 115.45      | 119.90   | 8      | 4     |
| 1   | A     | 12  | DG   | O4'-C1'-C2' | -8.87 | 98.80       | 105.90   | 8      | 2     |
| 2   | B     | 17  | DG   | N9-C4-C5    | -8.83 | 101.87      | 105.40   | 1      | 3     |
| 1   | A     | 11  | DG   | N3-C4-N9    | 8.75  | 131.25      | 126.00   | 6      | 3     |
| 1   | A     | 13  | DG   | C5-C6-O6    | 8.74  | 133.84      | 128.60   | 8      | 2     |
| 2   | B     | 22  | DT   | C5-C4-O4    | 8.70  | 130.99      | 124.90   | 7      | 3     |
| 2   | B     | 14  | DC   | O4'-C1'-N1  | 8.68  | 114.08      | 108.00   | 10     | 4     |
| 2   | B     | 16  | DC   | O4'-C4'-C3' | -8.67 | 100.80      | 106.00   | 2      | 4     |
| 1   | A     | 9   | DC   | C6-N1-C2    | -8.67 | 116.83      | 120.30   | 5      | 6     |
| 1   | A     | 3   | DA   | C8-N9-C4    | -8.67 | 102.33      | 105.80   | 7      | 3     |
| 2   | B     | 26  | DG   | O4'-C4'-C3' | -8.66 | 100.80      | 106.00   | 4      | 5     |
| 1   | A     | 8   | DA   | C5-N7-C8    | -8.63 | 99.58       | 103.90   | 4      | 6     |
| 2   | B     | 23  | DT   | C1'-O4'-C4' | -8.63 | 101.47      | 110.10   | 6      | 3     |
| 1   | A     | 13  | DG   | N3-C4-C5    | -8.56 | 124.32      | 128.60   | 9      | 4     |
| 2   | B     | 18  | DG   | C8-N9-C4    | -8.55 | 102.98      | 106.40   | 3      | 4     |
| 2   | B     | 26  | DG   | C6-N1-C2    | -8.55 | 119.97      | 125.10   | 8      | 1     |
| 2   | B     | 23  | DT   | N1-C2-O2    | 8.54  | 129.93      | 123.10   | 10     | 4     |
| 1   | A     | 6   | DG   | O4'-C4'-C3' | 8.53  | 111.12      | 106.00   | 3      | 3     |
| 1   | A     | 4   | DA   | C6-N1-C2    | -8.53 | 113.48      | 118.60   | 4      | 3     |
| 1   | A     | 1   | DC   | C5-C4-N4    | 8.52  | 126.16      | 120.20   | 7      | 3     |
| 2   | B     | 22  | DT   | C4-C5-C6    | 8.52  | 123.11      | 118.00   | 2      | 3     |
| 1   | A     | 5   | DA   | C6-C5-N7    | 8.51  | 138.26      | 132.30   | 7      | 2     |
| 1   | A     | 2   | DC   | C1'-O4'-C4' | -8.51 | 101.59      | 110.10   | 7      | 3     |
| 2   | B     | 20  | DC   | C5-C6-N1    | -8.51 | 116.75      | 121.00   | 10     | 4     |
| 1   | A     | 12  | DG   | C6-N1-C2    | -8.50 | 120.00      | 125.10   | 2      | 3     |
| 1   | A     | 11  | DG   | N9-C4-C5    | 8.49  | 108.80      | 105.40   | 2      | 5     |
| 2   | B     | 24  | DT   | C4-C5-C6    | 8.49  | 123.09      | 118.00   | 3      | 3     |
| 1   | A     | 9   | DC   | O4'-C4'-C3' | 8.49  | 111.09      | 106.00   | 10     | 3     |
| 2   | B     | 17  | DG   | N3-C4-C5    | -8.47 | 124.36      | 128.60   | 2      | 3     |
| 2   | B     | 20  | DC   | C5-C4-N4    | -8.39 | 114.33      | 120.20   | 3      | 3     |
| 1   | A     | 8   | DA   | C5-C6-N6    | 8.37  | 130.40      | 123.70   | 2      | 3     |
| 1   | A     | 5   | DA   | C4-C5-N7    | 8.34  | 114.87      | 110.70   | 8      | 1     |
| 2   | B     | 19  | DT   | O4'-C4'-C3' | -8.32 | 101.01      | 106.00   | 7      | 3     |
| 2   | B     | 19  | DT   | N3-C4-O4    | -8.28 | 114.93      | 119.90   | 3      | 2     |
| 2   | B     | 23  | DT   | O4'-C1'-C2' | -8.28 | 99.28       | 105.90   | 9      | 4     |
| 2   | B     | 23  | DT   | C4-C5-C7    | 8.27  | 123.96      | 119.00   | 3      | 4     |
| 2   | B     | 18  | DG   | C2-N3-C4    | 8.26  | 116.03      | 111.90   | 7      | 2     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 3   | DA   | C4-C5-N7    | 8.26  | 114.83      | 110.70   | 4      | 4     |
| 2   | B     | 18  | DG   | C5-C6-N1    | 8.25  | 115.62      | 111.50   | 6      | 3     |
| 2   | B     | 17  | DG   | C8-N9-C4    | -8.24 | 103.11      | 106.40   | 9      | 4     |
| 1   | A     | 8   | DA   | N7-C8-N9    | 8.24  | 117.92      | 113.80   | 4      | 3     |
| 1   | A     | 3   | DA   | C5-C6-N6    | 8.23  | 130.28      | 123.70   | 4      | 2     |
| 2   | B     | 17  | DG   | P-O3'-C3'   | 8.21  | 129.56      | 119.70   | 9      | 2     |
| 1   | A     | 11  | DG   | N3-C2-N2    | -8.21 | 114.15      | 119.90   | 2      | 3     |
| 2   | B     | 23  | DT   | P-O3'-C3'   | 8.18  | 129.52      | 119.70   | 3      | 3     |
| 1   | A     | 13  | DG   | C4'-C3'-C2' | -8.11 | 95.80       | 103.10   | 10     | 3     |
| 1   | A     | 3   | DA   | O4'-C1'-N9  | 8.06  | 113.64      | 108.00   | 6      | 3     |
| 2   | B     | 24  | DT   | C5-C4-O4    | 8.05  | 130.53      | 124.90   | 9      | 3     |
| 2   | B     | 26  | DG   | C4-C5-N7    | -8.04 | 107.58      | 110.80   | 3      | 3     |
| 2   | B     | 18  | DG   | C4-C5-C6    | -8.01 | 114.00      | 118.80   | 5      | 1     |
| 2   | B     | 24  | DT   | C2-N3-C4    | -8.00 | 122.40      | 127.20   | 5      | 4     |
| 2   | B     | 24  | DT   | C5-C6-N1    | -8.00 | 118.90      | 123.70   | 3      | 5     |
| 2   | B     | 25  | DG   | P-O3'-C3'   | 7.93  | 129.21      | 119.70   | 8      | 5     |
| 2   | B     | 19  | DT   | O5'-P-OP2   | -7.92 | 98.57       | 105.70   | 9      | 2     |
| 2   | B     | 23  | DT   | N3-C4-C5    | -7.91 | 110.46      | 115.20   | 4      | 3     |
| 1   | A     | 4   | DA   | C8-N9-C4    | -7.89 | 102.64      | 105.80   | 5      | 1     |
| 1   | A     | 6   | DG   | C5-C6-N1    | 7.88  | 115.44      | 111.50   | 5      | 2     |
| 1   | A     | 8   | DA   | C1'-O4'-C4' | -7.87 | 102.23      | 110.10   | 5      | 2     |
| 1   | A     | 12  | DG   | C5-N7-C8    | -7.82 | 100.39      | 104.30   | 6      | 6     |
| 1   | A     | 6   | DG   | C5-N7-C8    | -7.80 | 100.40      | 104.30   | 5      | 2     |
| 1   | A     | 11  | DG   | N1-C2-N3    | -7.80 | 119.22      | 123.90   | 1      | 3     |
| 1   | A     | 10  | DC   | C4-C5-C6    | -7.80 | 113.50      | 117.40   | 3      | 3     |
| 1   | A     | 10  | DC   | P-O3'-C3'   | 7.75  | 129.00      | 119.70   | 1      | 2     |
| 1   | A     | 4   | DA   | C4-C5-N7    | 7.74  | 114.57      | 110.70   | 1      | 2     |
| 2   | B     | 14  | DC   | C4-C5-C6    | 7.72  | 121.26      | 117.40   | 8      | 4     |
| 1   | A     | 11  | DG   | C3'-C2'-C1' | -7.71 | 93.25       | 102.50   | 7      | 2     |
| 2   | B     | 14  | DC   | C1'-O4'-C4' | -7.69 | 102.41      | 110.10   | 7      | 3     |
| 1   | A     | 5   | DA   | C5-C6-N6    | 7.65  | 129.82      | 123.70   | 2      | 1     |
| 1   | A     | 6   | DG   | N1-C2-N2    | 7.64  | 123.08      | 116.20   | 5      | 4     |
| 1   | A     | 5   | DA   | C2-N3-C4    | 7.64  | 114.42      | 110.60   | 5      | 4     |
| 1   | A     | 12  | DG   | C3'-C2'-C1' | 7.62  | 111.64      | 102.50   | 4      | 2     |
| 1   | A     | 11  | DG   | C5-C6-O6    | 7.60  | 133.16      | 128.60   | 9      | 4     |
| 2   | B     | 20  | DC   | O5'-P-OP1   | -7.60 | 98.86       | 105.70   | 10     | 1     |
| 2   | B     | 20  | DC   | C4-C5-C6    | -7.60 | 113.60      | 117.40   | 2      | 3     |
| 2   | B     | 18  | DG   | C6-C5-N7    | 7.59  | 134.96      | 130.40   | 5      | 1     |
| 2   | B     | 24  | DT   | C1'-O4'-C4' | -7.59 | 102.51      | 110.10   | 7      | 2     |
| 1   | A     | 3   | DA   | N9-C4-C5    | -7.57 | 102.77      | 105.80   | 8      | 2     |
| 1   | A     | 4   | DA   | N3-C4-N9    | -7.57 | 121.34      | 127.40   | 2      | 2     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 6   | DG   | C8-N9-C4    | -7.56 | 103.38      | 106.40   | 7      | 6     |
| 1   | A     | 13  | DG   | O5'-P-OP1   | -7.56 | 98.89       | 105.70   | 9      | 1     |
| 1   | A     | 13  | DG   | N1-C2-N2    | 7.55  | 123.00      | 116.20   | 9      | 2     |
| 1   | A     | 11  | DG   | C5-N7-C8    | 7.55  | 108.07      | 104.30   | 5      | 4     |
| 1   | A     | 5   | DA   | C5-N7-C8    | -7.55 | 100.12      | 103.90   | 10     | 2     |
| 2   | B     | 21  | DC   | P-O3'-C3'   | 7.54  | 128.75      | 119.70   | 6      | 3     |
| 2   | B     | 19  | DT   | N3-C4-C5    | -7.52 | 110.69      | 115.20   | 9      | 1     |
| 1   | A     | 13  | DG   | O4'-C1'-C2' | -7.51 | 99.89       | 105.90   | 8      | 3     |
| 2   | B     | 16  | DC   | C1'-O4'-C4' | -7.50 | 102.60      | 110.10   | 7      | 3     |
| 1   | A     | 6   | DG   | C6-C5-N7    | 7.48  | 134.89      | 130.40   | 4      | 2     |
| 1   | A     | 5   | DA   | N7-C8-N9    | 7.47  | 117.54      | 113.80   | 10     | 4     |
| 1   | A     | 10  | DC   | C1'-O4'-C4' | -7.46 | 102.64      | 110.10   | 3      | 2     |
| 2   | B     | 23  | DT   | N1-C2-N3    | 7.46  | 119.07      | 114.60   | 10     | 3     |
| 2   | B     | 18  | DG   | N3-C4-C5    | -7.44 | 124.88      | 128.60   | 6      | 3     |
| 1   | A     | 8   | DA   | N1-C2-N3    | -7.43 | 125.58      | 129.30   | 3      | 5     |
| 2   | B     | 26  | DG   | C5-C6-O6    | 7.41  | 133.04      | 128.60   | 1      | 5     |
| 1   | A     | 4   | DA   | N9-C4-C5    | 7.40  | 108.76      | 105.80   | 5      | 2     |
| 2   | B     | 17  | DG   | O4'-C1'-C2' | -7.40 | 99.98       | 105.90   | 7      | 2     |
| 2   | B     | 21  | DC   | C1'-O4'-C4' | -7.39 | 102.71      | 110.10   | 2      | 3     |
| 1   | A     | 3   | DA   | C6-C5-N7    | 7.38  | 137.47      | 132.30   | 2      | 1     |
| 1   | A     | 6   | DG   | C5-C6-O6    | 7.38  | 133.03      | 128.60   | 6      | 3     |
| 1   | A     | 2   | DC   | C5-C4-N4    | -7.37 | 115.04      | 120.20   | 7      | 3     |
| 1   | A     | 13  | DG   | N9-C1'-C2'  | -7.37 | 98.60       | 112.60   | 4      | 1     |
| 2   | B     | 18  | DG   | O4'-C1'-C2' | -7.35 | 100.02      | 105.90   | 2      | 4     |
| 1   | A     | 1   | DC   | C5-C6-N1    | -7.30 | 117.35      | 121.00   | 7      | 3     |
| 1   | A     | 10  | DC   | C5-C6-N1    | -7.23 | 117.39      | 121.00   | 6      | 3     |
| 1   | A     | 12  | DG   | N3-C2-N2    | 7.22  | 124.95      | 119.90   | 4      | 2     |
| 1   | A     | 11  | DG   | C4-C5-C6    | -7.20 | 114.48      | 118.80   | 4      | 3     |
| 1   | A     | 12  | DG   | C4'-C3'-C2' | -7.20 | 96.62       | 103.10   | 4      | 3     |
| 2   | B     | 25  | DG   | C5-C6-O6    | 7.20  | 132.92      | 128.60   | 2      | 2     |
| 2   | B     | 26  | DG   | N1-C2-N3    | 7.17  | 128.20      | 123.90   | 8      | 3     |
| 1   | A     | 13  | DG   | C2-N3-C4    | 7.17  | 115.48      | 111.90   | 5      | 2     |
| 2   | B     | 14  | DC   | C4'-C3'-C2' | -7.16 | 96.66       | 103.10   | 9      | 1     |
| 2   | B     | 19  | DT   | C3'-C2'-C1' | 7.15  | 111.08      | 102.50   | 8      | 3     |
| 1   | A     | 12  | DG   | N7-C8-N9    | 7.14  | 116.67      | 113.10   | 1      | 3     |
| 1   | A     | 9   | DC   | O4'-C1'-C2' | -7.13 | 100.19      | 105.90   | 9      | 4     |
| 1   | A     | 11  | DG   | C1'-O4'-C4' | -7.13 | 102.97      | 110.10   | 1      | 2     |
| 1   | A     | 9   | DC   | N1-C2-N3    | 7.07  | 124.15      | 119.20   | 5      | 5     |
| 1   | A     | 8   | DA   | P-O3'-C3'   | 7.00  | 128.10      | 119.70   | 2      | 6     |
| 2   | B     | 20  | DC   | P-O3'-C3'   | 6.99  | 128.08      | 119.70   | 7      | 2     |
| 2   | B     | 26  | DG   | C5-N7-C8    | -6.98 | 100.81      | 104.30   | 6      | 3     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 11  | DG   | C4'-C3'-C2' | -6.96 | 96.84       | 103.10   | 3      | 1     |
| 1   | A     | 2   | DC   | O4'-C1'-C2' | -6.94 | 100.35      | 105.90   | 8      | 3     |
| 1   | A     | 8   | DA   | O4'-C1'-C2' | -6.92 | 100.37      | 105.90   | 9      | 2     |
| 2   | B     | 17  | DG   | C4-C5-N7    | -6.92 | 108.03      | 110.80   | 2      | 4     |
| 2   | B     | 21  | DC   | N3-C4-N4    | -6.91 | 113.16      | 118.00   | 1      | 2     |
| 2   | B     | 18  | DG   | N7-C8-N9    | -6.91 | 109.65      | 113.10   | 2      | 3     |
| 2   | B     | 19  | DT   | P-O3'-C3'   | 6.91  | 127.99      | 119.70   | 2      | 3     |
| 1   | A     | 3   | DA   | C6-N1-C2    | -6.90 | 114.46      | 118.60   | 10     | 5     |
| 1   | A     | 5   | DA   | C8-N9-C4    | -6.90 | 103.04      | 105.80   | 3      | 2     |
| 2   | B     | 26  | DG   | C6-C5-N7    | 6.89  | 134.53      | 130.40   | 5      | 4     |
| 1   | A     | 8   | DA   | N3-C4-C5    | 6.88  | 131.62      | 126.80   | 7      | 1     |
| 2   | B     | 16  | DC   | C4'-C3'-C2' | -6.87 | 96.91       | 103.10   | 10     | 1     |
| 1   | A     | 12  | DG   | P-O3'-C3'   | 6.87  | 127.94      | 119.70   | 2      | 2     |
| 1   | A     | 11  | DG   | P-O3'-C3'   | 6.85  | 127.92      | 119.70   | 2      | 3     |
| 1   | A     | 3   | DA   | C2-N3-C4    | 6.80  | 114.00      | 110.60   | 7      | 6     |
| 2   | B     | 17  | DG   | C3'-C2'-C1' | 6.79  | 110.65      | 102.50   | 7      | 1     |
| 2   | B     | 26  | DG   | N9-C4-C5    | 6.78  | 108.11      | 105.40   | 3      | 3     |
| 2   | B     | 15  | DC   | C3'-C2'-C1' | 6.76  | 110.62      | 102.50   | 3      | 1     |
| 2   | B     | 16  | DC   | N1-C2-N3    | 6.72  | 123.91      | 119.20   | 2      | 2     |
| 1   | A     | 12  | DG   | N1-C2-N2    | 6.68  | 122.22      | 116.20   | 3      | 1     |
| 1   | A     | 9   | DC   | C4'-C3'-C2' | 6.68  | 109.12      | 103.10   | 7      | 3     |
| 1   | A     | 12  | DG   | C1'-O4'-C4' | -6.66 | 103.44      | 110.10   | 7      | 1     |
| 2   | B     | 23  | DT   | O5'-P-OP1   | -6.63 | 99.73       | 105.70   | 6      | 1     |
| 1   | A     | 2   | DC   | N1-C2-N3    | 6.61  | 123.83      | 119.20   | 1      | 3     |
| 1   | A     | 6   | DG   | O4'-C1'-C2' | 6.60  | 111.18      | 105.90   | 1      | 4     |
| 1   | A     | 11  | DG   | O4'-C1'-C2' | 6.58  | 111.16      | 105.90   | 6      | 1     |
| 2   | B     | 22  | DT   | O4'-C1'-C2' | -6.58 | 100.64      | 105.90   | 4      | 2     |
| 2   | B     | 24  | DT   | N3-C4-C5    | 6.56  | 119.14      | 115.20   | 5      | 2     |
| 1   | A     | 4   | DA   | P-O3'-C3'   | 6.56  | 127.57      | 119.70   | 6      | 2     |
| 1   | A     | 4   | DA   | N3-C4-C5    | 6.53  | 131.37      | 126.80   | 2      | 1     |
| 2   | B     | 26  | DG   | N1-C2-N2    | 6.53  | 122.07      | 116.20   | 5      | 2     |
| 1   | A     | 10  | DC   | N1-C2-N3    | 6.52  | 123.77      | 119.20   | 4      | 1     |
| 2   | B     | 26  | DG   | O5'-P-OP1   | 6.46  | 118.46      | 110.70   | 8      | 1     |
| 2   | B     | 23  | DT   | C3'-C2'-C1' | 6.44  | 110.23      | 102.50   | 1      | 2     |
| 1   | A     | 6   | DG   | C1'-O4'-C4' | -6.42 | 103.68      | 110.10   | 1      | 1     |
| 2   | B     | 21  | DC   | C6-N1-C2    | -6.40 | 117.74      | 120.30   | 9      | 4     |
| 1   | A     | 4   | DA   | C5-N7-C8    | 6.39  | 107.10      | 103.90   | 8      | 2     |
| 2   | B     | 26  | DG   | C5'-C4'-C3' | 6.38  | 125.58      | 114.10   | 1      | 1     |
| 1   | A     | 5   | DA   | O4'-C1'-C2' | -6.38 | 100.80      | 105.90   | 10     | 2     |
| 1   | A     | 13  | DG   | OP1-P-OP2   | -6.38 | 110.03      | 119.60   | 3      | 1     |
| 1   | A     | 1   | DC   | P-O3'-C3'   | 6.37  | 127.34      | 119.70   | 10     | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 2   | B     | 17  | DG   | C1'-O4'-C4' | -6.33 | 103.77      | 110.10   | 1      | 1     |
| 1   | A     | 11  | DG   | N1-C2-N2    | 6.33  | 121.90      | 116.20   | 7      | 1     |
| 2   | B     | 24  | DT   | O4'-C1'-C2' | -6.32 | 100.85      | 105.90   | 10     | 4     |
| 1   | A     | 4   | DA   | C4'-C3'-C2' | -6.31 | 97.42       | 103.10   | 4      | 3     |
| 1   | A     | 5   | DA   | O4'-C1'-N9  | -6.30 | 103.59      | 108.00   | 6      | 1     |
| 2   | B     | 26  | DG   | C8-N9-C4    | -6.29 | 103.88      | 106.40   | 9      | 3     |
| 2   | B     | 19  | DT   | N1-C2-O2    | 6.29  | 128.13      | 123.10   | 8      | 4     |
| 1   | A     | 6   | DG   | C3'-C2'-C1' | -6.28 | 94.97       | 102.50   | 4      | 1     |
| 1   | A     | 12  | DG   | N1-C2-N3    | 6.26  | 127.66      | 123.90   | 5      | 4     |
| 2   | B     | 18  | DG   | C4'-C3'-C2' | -6.26 | 97.47       | 103.10   | 8      | 1     |
| 2   | B     | 22  | DT   | P-O3'-C3'   | 6.25  | 127.20      | 119.70   | 7      | 3     |
| 1   | A     | 4   | DA   | C5-C6-N6    | 6.25  | 128.70      | 123.70   | 10     | 3     |
| 2   | B     | 16  | DC   | C3'-C2'-C1' | 6.22  | 109.97      | 102.50   | 10     | 2     |
| 1   | A     | 12  | DG   | N3-C4-N9    | 6.20  | 129.72      | 126.00   | 6      | 2     |
| 1   | A     | 12  | DG   | N9-C1'-C2'  | -6.11 | 100.99      | 112.60   | 7      | 1     |
| 1   | A     | 8   | DA   | C4'-C3'-C2' | -6.10 | 97.61       | 103.10   | 5      | 3     |
| 1   | A     | 4   | DA   | N7-C8-N9    | -6.10 | 110.75      | 113.80   | 8      | 1     |
| 2   | B     | 25  | DG   | OP2-P-O3'   | 6.03  | 118.47      | 105.20   | 6      | 1     |
| 2   | B     | 18  | DG   | C1'-O4'-C4' | -6.03 | 104.07      | 110.10   | 8      | 2     |
| 1   | A     | 5   | DA   | N3-C4-N9    | -6.02 | 122.58      | 127.40   | 2      | 1     |
| 1   | A     | 2   | DC   | P-O3'-C3'   | 6.02  | 126.92      | 119.70   | 3      | 4     |
| 2   | B     | 25  | DG   | N3-C4-N9    | 6.02  | 129.61      | 126.00   | 2      | 1     |
| 2   | B     | 22  | DT   | C6-N1-C2    | -6.00 | 118.30      | 121.30   | 7      | 2     |
| 2   | B     | 21  | DC   | C5-C6-N1    | -6.00 | 118.00      | 121.00   | 4      | 1     |
| 1   | A     | 2   | DC   | C6-N1-C1'   | 5.99  | 127.98      | 120.80   | 10     | 1     |
| 2   | B     | 17  | DG   | C5-C6-O6    | 5.96  | 132.18      | 128.60   | 10     | 2     |
| 2   | B     | 14  | DC   | N1-C2-N3    | 5.95  | 123.37      | 119.20   | 8      | 3     |
| 2   | B     | 26  | DG   | C2-N3-C4    | 5.95  | 114.88      | 111.90   | 7      | 1     |
| 2   | B     | 21  | DC   | C3'-C2'-C1' | 5.94  | 109.63      | 102.50   | 1      | 3     |
| 2   | B     | 25  | DG   | O4'-C1'-C2' | -5.93 | 101.16      | 105.90   | 7      | 1     |
| 2   | B     | 17  | DG   | C4-C5-C6    | -5.92 | 115.25      | 118.80   | 8      | 1     |
| 2   | B     | 19  | DT   | O4'-C1'-C2' | -5.91 | 101.17      | 105.90   | 5      | 2     |
| 2   | B     | 25  | DG   | C4-C5-C6    | -5.89 | 115.26      | 118.80   | 9      | 2     |
| 1   | A     | 13  | DG   | C8-N9-C1'   | 5.88  | 134.64      | 127.00   | 10     | 1     |
| 1   | A     | 1   | DC   | C1'-O4'-C4' | -5.86 | 104.24      | 110.10   | 5      | 1     |
| 1   | A     | 13  | DG   | N3-C4-N9    | 5.84  | 129.51      | 126.00   | 4      | 1     |
| 1   | A     | 6   | DG   | C4-C5-C6    | -5.84 | 115.30      | 118.80   | 5      | 1     |
| 2   | B     | 23  | DT   | C2-N3-C4    | -5.84 | 123.70      | 127.20   | 7      | 3     |
| 1   | A     | 13  | DG   | P-O5'-C5'   | 5.83  | 130.23      | 120.90   | 6      | 1     |
| 1   | A     | 12  | DG   | OP1-P-O3'   | -5.80 | 92.43       | 105.20   | 6      | 1     |
| 2   | B     | 18  | DG   | C5-N7-C8    | -5.80 | 101.40      | 104.30   | 7      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 5   | DA   | N9-C4-C5    | 5.80  | 108.12      | 105.80   | 5      | 1     |
| 2   | B     | 24  | DT   | C4-C5-C7    | 5.78  | 122.47      | 119.00   | 10     | 1     |
| 1   | A     | 5   | DA   | C3'-C2'-C1' | -5.78 | 95.56       | 102.50   | 3      | 1     |
| 2   | B     | 24  | DT   | P-O5'-C5'   | 5.74  | 130.09      | 120.90   | 7      | 1     |
| 1   | A     | 10  | DC   | C3'-C2'-C1' | 5.72  | 109.37      | 102.50   | 6      | 1     |
| 2   | B     | 18  | DG   | N1-C2-N2    | 5.71  | 121.33      | 116.20   | 3      | 1     |
| 2   | B     | 24  | DT   | N1-C2-O2    | -5.67 | 118.56      | 123.10   | 4      | 2     |
| 2   | B     | 14  | DC   | O4'-C1'-C2' | -5.67 | 101.36      | 105.90   | 9      | 1     |
| 2   | B     | 19  | DT   | C6-N1-C1'   | -5.67 | 111.90      | 120.40   | 2      | 1     |
| 2   | B     | 26  | DG   | C3'-C2'-C1' | -5.64 | 95.73       | 102.50   | 4      | 1     |
| 2   | B     | 17  | DG   | C4-N9-C1'   | -5.64 | 119.17      | 126.50   | 4      | 1     |
| 1   | A     | 4   | DA   | C5'-C4'-O4' | 5.63  | 120.00      | 109.30   | 10     | 2     |
| 2   | B     | 25  | DG   | C1'-O4'-C4' | -5.59 | 104.51      | 110.10   | 3      | 2     |
| 2   | B     | 18  | DG   | N1-C2-N3    | 5.56  | 127.24      | 123.90   | 3      | 1     |
| 1   | A     | 5   | DA   | C1'-O4'-C4' | -5.51 | 104.59      | 110.10   | 6      | 2     |
| 1   | A     | 10  | DC   | P-O5'-C5'   | 5.51  | 129.72      | 120.90   | 9      | 1     |
| 2   | B     | 24  | DT   | P-O3'-C3'   | 5.49  | 126.29      | 119.70   | 10     | 1     |
| 1   | A     | 5   | DA   | N3-C4-C5    | 5.48  | 130.64      | 126.80   | 2      | 1     |
| 1   | A     | 3   | DA   | C1'-O4'-C4' | -5.47 | 104.62      | 110.10   | 10     | 2     |
| 1   | A     | 13  | DG   | C6-C5-N7    | 5.47  | 133.68      | 130.40   | 6      | 1     |
| 2   | B     | 16  | DC   | P-O3'-C3'   | 5.46  | 126.25      | 119.70   | 9      | 4     |
| 2   | B     | 26  | DG   | C4'-C3'-C2' | 5.46  | 108.02      | 103.10   | 3      | 1     |
| 1   | A     | 3   | DA   | C3'-C2'-C1' | -5.46 | 95.95       | 102.50   | 10     | 1     |
| 1   | A     | 9   | DC   | C3'-C2'-C1' | -5.44 | 95.97       | 102.50   | 6      | 1     |
| 1   | A     | 6   | DG   | C8-N9-C1'   | 5.43  | 134.06      | 127.00   | 9      | 1     |
| 1   | A     | 1   | DC   | C4'-C3'-C2' | 5.43  | 107.98      | 103.10   | 10     | 1     |
| 2   | B     | 19  | DT   | O5'-P-OP1   | 5.42  | 117.20      | 110.70   | 4      | 1     |
| 2   | B     | 17  | DG   | C8-N9-C1'   | 5.42  | 134.04      | 127.00   | 7      | 2     |
| 2   | B     | 15  | DC   | O5'-P-OP2   | -5.40 | 100.84      | 105.70   | 8      | 1     |
| 2   | B     | 24  | DT   | C5'-C4'-O4' | 5.37  | 119.50      | 109.30   | 8      | 1     |
| 2   | B     | 17  | DG   | C6-C5-N7    | 5.36  | 133.62      | 130.40   | 8      | 1     |
| 1   | A     | 6   | DG   | N3-C4-N9    | 5.36  | 129.22      | 126.00   | 3      | 2     |
| 1   | A     | 12  | DG   | C4'-C3'-O3' | -5.32 | 96.41       | 109.70   | 7      | 1     |
| 2   | B     | 21  | DC   | O4'-C1'-C2' | -5.31 | 101.65      | 105.90   | 5      | 1     |
| 2   | B     | 19  | DT   | OP2-P-O3'   | 5.29  | 116.85      | 105.20   | 10     | 1     |
| 2   | B     | 22  | DT   | C1'-O4'-C4' | 5.28  | 115.38      | 110.10   | 4      | 1     |
| 1   | A     | 3   | DA   | N7-C8-N9    | 5.26  | 116.43      | 113.80   | 7      | 1     |
| 1   | A     | 2   | DC   | C4'-C3'-C2' | 5.25  | 107.83      | 103.10   | 9      | 1     |
| 2   | B     | 23  | DT   | C6-N1-C2    | 5.24  | 123.92      | 121.30   | 4      | 1     |
| 1   | A     | 10  | DC   | C4'-C3'-C2' | -5.24 | 98.39       | 103.10   | 6      | 2     |
| 1   | A     | 4   | DA   | O4'-C1'-C2' | -5.23 | 101.72      | 105.90   | 7      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 2   | B     | 18  | DG   | N3-C4-N9    | -5.22 | 122.87      | 126.00   | 5      | 3     |
| 2   | B     | 16  | DC   | C5-C6-N1    | -5.21 | 118.39      | 121.00   | 2      | 3     |
| 1   | A     | 3   | DA   | P-O3'-C3'   | 5.17  | 125.90      | 119.70   | 2      | 2     |
| 1   | A     | 1   | DC   | N1-C1'-C2'  | -5.17 | 102.78      | 112.60   | 4      | 1     |
| 1   | A     | 1   | DC   | C2-N1-C1'   | 5.16  | 124.47      | 118.80   | 1      | 1     |
| 2   | B     | 19  | DT   | C1'-O4'-C4' | -5.15 | 104.95      | 110.10   | 8      | 1     |
| 1   | A     | 10  | DC   | O4'-C1'-C2' | -5.15 | 101.78      | 105.90   | 4      | 1     |
| 2   | B     | 15  | DC   | P-O3'-C3'   | 5.13  | 125.86      | 119.70   | 5      | 3     |
| 2   | B     | 20  | DC   | N1-C2-N3    | 5.11  | 122.78      | 119.20   | 1      | 1     |
| 1   | A     | 6   | DG   | C4-N9-C1'   | -5.10 | 119.87      | 126.50   | 9      | 1     |
| 1   | A     | 11  | DG   | N9-C1'-C2'  | 5.08  | 122.25      | 112.60   | 10     | 1     |
| 1   | A     | 13  | DG   | C1'-O4'-C4' | -5.08 | 105.02      | 110.10   | 8      | 1     |
| 2   | B     | 16  | DC   | C5-C4-N4    | 5.07  | 123.75      | 120.20   | 2      | 1     |
| 2   | B     | 24  | DT   | OP2-P-O3'   | 5.06  | 116.33      | 105.20   | 10     | 1     |
| 2   | B     | 15  | DC   | O4'-C4'-C3' | 5.03  | 109.02      | 106.00   | 7      | 1     |
| 2   | B     | 25  | DG   | N1-C2-N2    | -5.03 | 111.67      | 116.20   | 6      | 1     |
| 1   | A     | 13  | DG   | C4-N9-C1'   | -5.02 | 119.97      | 126.50   | 10     | 1     |
| 2   | B     | 14  | DC   | P-O3'-C3'   | 5.02  | 125.72      | 119.70   | 2      | 1     |
| 2   | B     | 23  | DT   | OP1-P-OP2   | -5.00 | 112.09      | 119.60   | 9      | 1     |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 11  | DG   | Sidechain | 9              |
| 2   | B     | 26  | DG   | Sidechain | 8              |
| 2   | B     | 17  | DG   | Sidechain | 8              |
| 1   | A     | 6   | DG   | Sidechain | 8              |
| 2   | B     | 18  | DG   | Sidechain | 8              |
| 1   | A     | 13  | DG   | Sidechain | 7              |
| 2   | B     | 24  | DT   | Sidechain | 7              |
| 2   | B     | 20  | DC   | Sidechain | 7              |
| 2   | B     | 25  | DG   | Sidechain | 6              |
| 2   | B     | 15  | DC   | Sidechain | 6              |
| 1   | A     | 8   | DA   | Sidechain | 6              |
| 1   | A     | 2   | DC   | Sidechain | 5              |
| 1   | A     | 12  | DG   | Sidechain | 5              |
| 2   | B     | 19  | DT   | Sidechain | 5              |
| 1   | A     | 4   | DA   | Sidechain | 4              |
| 2   | B     | 14  | DC   | Sidechain | 4              |

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| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 2   | B     | 16  | DC   | Sidechain | 4              |
| 1   | A     | 1   | DC   | Sidechain | 4              |
| 2   | B     | 23  | DT   | Sidechain | 3              |
| 2   | B     | 22  | DT   | Sidechain | 3              |
| 2   | B     | 21  | DC   | Sidechain | 2              |
| 1   | A     | 10  | DC   | Sidechain | 2              |
| 1   | A     | 5   | DA   | Sidechain | 2              |
| 1   | A     | 9   | DC   | Sidechain | 1              |

## 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All   | 5687  | 3201     | 3071     | -       |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 1   | AAB  | A     | 7   | 1    | 8,12,13      | 1.45±0.51 | 0±0 (1±3%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 1   | AAB  | A     | 7   | 1    | 10,16,19    | 1.46±0.35 | 0±0 (0±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings     |
|-----|------|-------|-----|------|---------|-------------|-----------|
| 1   | AAB  | A     | 7   | 1    | -       | 0±0,3,17,18 | 0±0,1,1,1 |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
|     |       |     |      |         |      |             |          | Worst  | Total |
| 1   | A     | 7   | AAB  | C2'-C1' | 6.19 | 1.61        | 1.52     | 6      | 1     |

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided